Density of states for the gravitational field in black-hole topologies

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Using a previously developed formulation of black-hole thermodynamics for a system of finite size, we show that the partition function of the related canonical ensemble *can* be used to obtain the density of states in the microcanonical ensemble. We work with the partition function in a zero-loop approximation based on classical solutions with fixed boundary data and obtain the corresponding density of states by using an inverse Laplace transform. The computation requires the introduction of a uniformizing variable so that a path can be defined along which the classical action of a stable black hole is single valued in the integration over imaginary inverse temperatures. Although the zero-loop partition function is not a Laplace transform, its inversion integral yielding the density of states is nevertheless well defined, and we show that it is the exact inverse of a Fourier-Laplace integration over all real energies, positive and negative. We argue that (1) this need for all positive and negative energies and (2) a constraint on the boundary data for obtaining the partition function from classical solutions are both consequences of the zero-loop approximation that should be absent in a complete quantum theory. We also find that the single-valued action enables a discussion of negative temperatures for positive mean energies that appear to be essential for a satisfactory relation between the partition function and the density of states in the zero-loop approximation. The full significance of this observation must await further study.

I. INTRODUCTION

The association of a temperature with the surface gravity of a black hole[1] and an entropy with the area of its event horizon[2] brought to an end several years of speculation about the relation between black-hole physics and thermodynamics and led to the steady development of black-hole thermodynamics. Though originally conceived for black holes in asymptotically flat or de Sitter spaces of infinite extent, this study is formulated more precisely for black holes in spaces of finite extent.[3] In particular, it is then possible to give a complete thermodynamic description of the canonical ensemble for a classical black hole in thermal equilibrium at temperature $T=\beta^{-1}$ with the walls of a spherical box having finite proper area $A=4\pi r_0{}^2$. In this paper, following earlier work,[4,5] we reexamine the question of determining the density of states of the microcanonical ensemble for a black hole in a thermally isolated box containing a fixed amount of energy E. In fact, in this form the question involves slightly inexact terminology. Therefore, we shall first reformulate the question, then turn a suitable approximation for the physical description into a well-defined mathematical problem which we solve, and, finally, show that there is an interesting regime in which the mathematical solution has a sensible physical interpretation.

For systems involving the gravitational field, as in any quantum-field-theoretic treatment of statistical mechanics, a convenient starting point in discussing the canonical ensemble is the partition function expressed as a Euclidean path integral:

$$Z(\beta)=\int d[g]\exp(-\hbar^{-1}I[g]) \ , \tag{1.1}$$

where the sum is over all real Euclidean metrics on manifolds M with fixed boundary ∂M. We shall consider the boundary topology $S^1\times S^2$ with the S^1 being a round metric circle of proper circumference $\beta\hbar$ and the S^2 a standard metric sphere of area $A=4\pi r_0{}^2$. This fixing of the topology and the metric three-geometry of the boundary is not only part of the definition of the canonical ensemble we shall be working with, but is also precisely the condition[3,6] which ensures that classical solutions are local extrema of the Euclidean action I, a point that will prove essential in what follows. Because the partition function can be regarded formally as a Laplace transform of the density of states, once the partition function has been calculated by independent means, the most direct way to obtain the density of states is by using an inverse Laplace transform:

$$\nu(E)=\frac{1}{2\pi i}\int_{-i\infty+c}^{i\infty+c} d\beta\, Z(\beta)\exp(\beta E) \ . \tag{1.2}$$

Actually, we shall be working only with a convenient approximation to the exact partition function (1.1) for gravitational thermodynamics. Setting aside, to begin with, the fact that our approximation cannot be a Laplace transform, we nevertheless proceed to evaluate the inversion integral and to determine the specification of the Fourier-Laplace transform of which it *is* an exact inverse.

Practical computations of path integrals often involve reducing the effective number of degrees of freedom in the integration to some very small number. In one variable, for example, the integral might then be approximated by taking a steepest-descent path through the saddle points of the exponent, the latter regarded as a function of a complexified variable. In path integrals, a stationary point of the action will become a saddle point for a path of steepest descent only if the corresponding classical solution is stable, meaning that its action is a local minimum, not just a local extremum. In quantum field theory, the action of the classical solution is usually ignored while integration along a path of steepest descent is regarded as a one-loop calculation. In the case of gravity, however, the classical action definitely cannot be ignored. In fact, for systems far from the Planck regime, one can argue that the path integral for the partition function will be entirely dominated by contributions from the stable classical solutions which comprise the local minima of the gravitational action. Dropping even the one-loop corrections from integration along the paths of steepest descent, one can than adopt a zero-loop approximation

$$Z_0(\beta)\approx\sum\exp(-\hbar^{-1}\mathrm{I}_{\mathrm{classical,stable}}) \tag{1.3}$$

as an operational starting point for gravitational thermodynamics. Indeed, this has been the basis of a previous discussion[3] of black-hole thermodynamics, with

$$\hbar^{-1}\mathrm{I}_{\mathrm{classical,stable}}=\beta F \ , \tag{1.4}$$

where F is the Helmholtz free energy. Although Z_0 is determined by the action evaluated at classical solutions, we nevertheless refer to (1.3) as a semiclassical approximation, since it does not survive in the classical limit.

In flat-space quantum field theory, the path integral may include topological distinct gauge-field sectors, while in the case of gravity it will unavoidably include manifolds corresponding to different spacetime topologies. Given the state of uncertainty about how topology change might be effected in quantum gravity, it seems necessary for the present that different topological sectors be treated separately. For four-dimensional Riemannian manifolds, there are two topological invariants[7] expressible as integrals of the curvature: the Euler characteristic χ and the Hirzebruch signature τ. However, no systematic method is known to obtain all stationary points of the gravitational action for a specified topology with fixed boundary. Only through imposing isometries is it possible to construct any classical solutions explicitly. For a given topological sector, our attention will be focused on such known classical solutions.

For our discussion it is essential to realize that the usual manifold of flat space at finite temperatures, $S^1\times R^3$, with periodically identified Euclidean time, has Euler characteristic $\chi=0$, whereas the regular Euclidean black hole has topology $S^2\times R^2$ and $\chi=2$. Thus, although both manifolds have signature $\tau=0$, they belong to different topological sectors. Since the contribution of flat space in the $\chi=0$ sector can already be reasonably well understood (for example, even the one-loop contributions from thermal gravitons can be calculated), emphasis to date in gravitational thermodynamics has concentrated on the contribution of black holes in the $\chi=2$ ($\tau=0$) sector, especially because there are indeed nontrivial effects at zero loops from the classical action. It is to this contribution that we now turn.

II. THE CANONICAL ENSEMBLE

The Euclidean action for Einstein gravity is[4,8]

$$I=-\frac{1}{16\pi G}\int_M \sqrt{g}R\,d^4x+\frac{1}{8\pi G}\oint_{\partial M}\sqrt{\gamma}(K-K_0)d^3x \ , \tag{2.1}$$

which is stationary for four-metrics g which satisfy the Einstein equation with fixed three-geometry γ on the boundary ∂M. For flat space the classical action is zero while, in quadratic order, fluctuations around this background give the one-loop contribution of thermal gravitons. This is identical to the familiar result for the canonical ensemble of radiation in a box and up to small corrections arising from boundary effects is given by

$$\ln Z_1=\frac{1}{2160}\left[\frac{4\pi r_0}{\beta\hbar}\right]^3 . \tag{2.2}$$

The Euclidean black-hole solutions are given by the Schwarzschild metric

$$ds^2=\left[1-\frac{2GM}{r}\right]d\tau^2+\left[1-\frac{2GM}{r}\right]^{-1}dr^2+r^2d\Omega^2 \ , \tag{2.3}$$

where $\tau(4GM)^{-1}$ has period 2π and $d\Omega^2$ is the metric on the unit two-sphere. The mass M must be chosen to satisfy the boundary conditions of fixed β and r_0. These quantities are related by the Hawking temperature formula, which we express as

$$\frac{\beta\hbar}{4\pi r_0}=\frac{2GM}{r_0}\left[1-\frac{2GM}{r_0}\right]^{1/2}=\frac{r_+}{r_0}\left[1-\frac{r_+}{r_0}\right]^{1/2} , \tag{2.4}$$

where $r_+\equiv 2GM$ is the gravitational radius of the Schwarzschild black hole. The action expressed in terms of these variables is[3]

$$\begin{aligned}I&=12\pi GM^2-8\pi Mr_0\left[1-\left[1-\frac{2GM}{r_0}\right]^{1/2}\right]\\&=\frac{1}{G}\left\{3\pi r_+{}^2-4\pi r_+r_0\left[1-\left[1-\frac{r_+}{r_0}\right]^{1/2}\right]\right\}.\end{aligned} \tag{2.5}$$

Neither $I(M,r_0)$ nor the corresponding $I(\beta,r_0)$ is single valued, a problem which we treat in the next section.

It is of fundamental importance that real Euclidean black-hole geometries extremize the action only if the boundary data r_0 and β satisfy[3]

$$\frac{4\pi r_0}{\beta\hbar}\geq\frac{3\sqrt{3}}{2} . \tag{2.6}$$

When inequality holds, there are two positive solutions of (2.4) for the mass M. The lighter mass $M_1(\beta,r_0)<r_0(3G)^{-1}$ is an unstable equilibrium point

while the heavier mass $M_2(\beta,r_0)>r_0(3G)^{-1}$ is thermodynamically stable for the canonical ensemble defined by r_0 and β. In the limit $M_2-M_1\rightarrow 0$, or $M\rightarrow r_0(3G)^{-1}$, the unstable circular photon orbits coincide with the boundary of the box. The heavier mass black hole has a positive heat capacity, real energy fluctuations, and a smaller action than the lighter-mass black hole. In fact, for

$$\frac{4\pi r_0}{\beta\hbar}>\frac{27}{8}\ , \tag{2.7}$$

the action of the heavier-mass black hole is negative, leading to a smaller zero-loop free energy than that of flat space, an observation central to any discussion of phase transitions in gravitational thermodynamics.

Finally, we note that in the black-hole sector, we have, from the thermodynamic definitions for the canonical ensemble, with $M=M_2$ in r_+ and with r_0 fixed,

$$\langle E\rangle\approx\frac{-\partial\ln Z_0}{\partial\beta}=\frac{r_0}{G}\left[1-\left[1-\frac{r_+}{r_0}\right]^{1/2}\right]\ , \tag{2.8}$$

$$S\approx\beta\langle E\rangle+\ln Z_0=\pi\left[\frac{r_+}{r_p}\right]^2\ , \tag{2.9}$$

and

$$\langle(\Delta E)^2\rangle\approx\frac{1}{Z_0}\frac{\partial^2 Z_0}{\partial\beta^2}-\left[\frac{\partial\ln Z_0}{\partial\beta}\right]^2$$
$$=\frac{\hbar}{8\pi G}\left[\frac{3r_+}{2r_0}-1\right]^{-1}\ , \tag{2.10}$$

where $r_p=(G\hbar)^{1/2}$ is the Planck length. A particularly important consequence of (2.8) is that

$$M=\langle E\rangle-\frac{1}{2}\frac{G\langle E\rangle^2}{r_0}\ , \tag{2.11}$$

that is, the Schwarzschild mass is the thermal energy plus the gravitational self-energy. For systems which contain a stable black hole we have

$$\left[1-\frac{1}{\sqrt{3}}\right]<\frac{G\langle E\rangle}{r_0}<1\ , \tag{2.12}$$

which determines what we shall refer to as the "physical" range for the energy of a black hole in a box. We also note for later use that (2.4), (2.6), and the constraints for the existence of stable equilibrium, require r_+ to satisfy

$$\frac{2}{3}<\frac{r_+}{r_0}<1\ . \tag{2.13}$$

Thus, in particular, one can see from (2.10) that energy fluctuations are *always* of the order of the Planck mass (r_pG^{-1}), except in the limit $r_+\rightarrow 2r_0/3$.

III. A SINGLE-VALUED ACTION

In this section we introduce a change of variables in terms of which both the action and the inverse temperature become single valued. This is essential in order to have a well-defined partition function and is also required for an unambiguous specification of the contour of integration in our subsequent computation of the density of states. It will be convenient to replace the inverse temperature β with the dimensionless quantity

$$\sigma=\frac{\beta\hbar}{4\pi r_0}\ , \tag{3.1}$$

which has already appeared in (2.2), (2.6), and (2.7). Because the branch cut for the r_+ dependence is identical in the inverse temperature (2.4) and in the action (2.5), the single new variable

$$\zeta=i\left[1-\frac{r_+}{r_0}\right]^{1/2}\ , \tag{3.2}$$

allows us to express both the action and the inverse temperature as the single-valued functions

$$I=\frac{4\pi r_0^{\,2}}{G}\left[\tfrac{1}{4}(3\zeta^4+2\zeta^2-1)-i\zeta(1+\zeta^2)\right] \tag{3.3}$$

and

$$\sigma=-i\zeta(1+\zeta^2)\ . \tag{3.4}$$

These forms enable us to integrate over imaginary σ once we determine how to choose a contour in the complex ζ plane. We see from (3.2) that for black holes with real positive mass, ζ must be imaginary. Condition (2.13) for stable thermal equilibrium requires ζ to satisfy

$$0<-i\zeta<\frac{1}{\sqrt{3}}\ , \tag{3.5}$$

whereas for the unstable stationary point for the gravitational action of a black hole, we have

$$\frac{1}{\sqrt{3}}<-i\zeta<1\ . \tag{3.6}$$

The map in (3.4) has two critical points $\zeta=\pm i(3)^{-1/2}$. We choose the complex σ plane to be cut from the images of these critical points at $\sigma=\pm 2(27)^{-1/2}$ to $\pm\infty$, respectively. These cuts divide the ζ plane into three regions as delineated by the thick lines shown in Fig. 1. The upper and lower regions we denote as regions II and III, respectively, with the region in between being designated as region I. The action and the partition function behave differently in each of these regions. The inverse map for the imaginary σ axis gives three lines in the complex ζ plane, namely, the real ζ axis in region I, and in regions II and III the lines given by $\zeta=u+iv$ with

$$v^2=1+3u^2\ . \tag{3.7}$$

The $\mathrm{Re}(\sigma)<0$ sides of these lines are hatched on Fig. 1 in each case. The cut σ plane and a number of details on it are shown in Fig. 2. In the integral for the density of states, the integrand is well behaved as $\sigma\rightarrow\pm i\infty$ only for those σ that are images of points ζ in region I. It is precisely this region which maps to the real inverse temperatures of stable black holes; that is, it is only in this region that we have stable equilibrium with which to compute the partition function. Therefore, our choice of

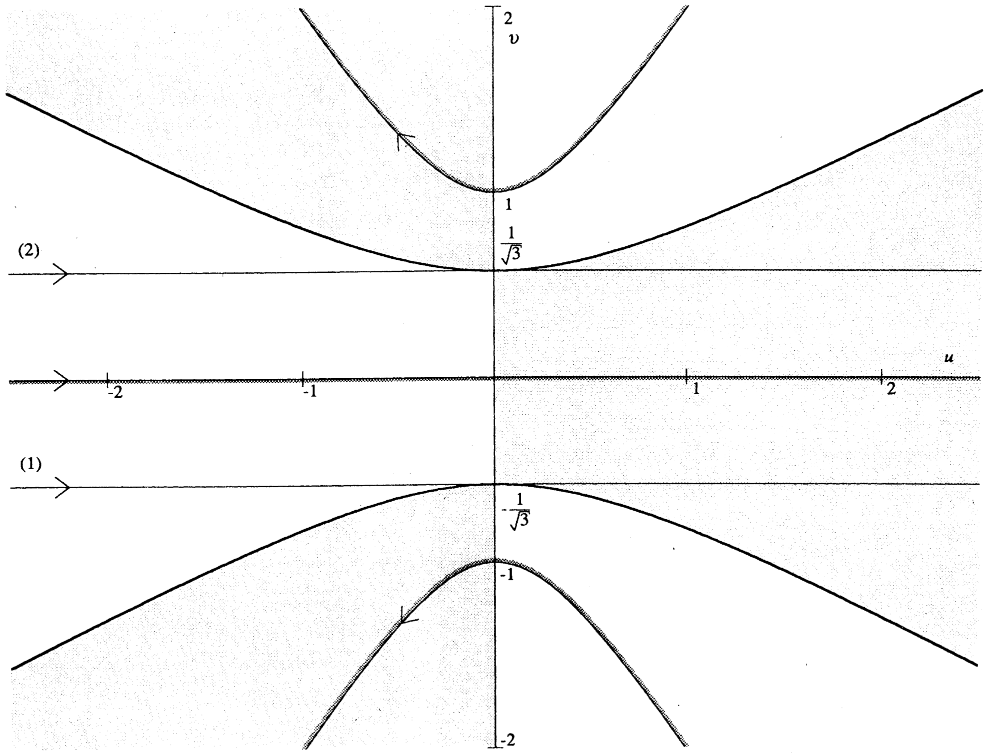

FIG. 1. The complex plane for $\zeta = u + iv$, the variable in terms of which the action and the inverse temperature become single valued. This plane has been divided into three regions by the two thick lines, $3v^2 = 1 + u^2$, which map to cuts in the complex σ plane (see Fig. 2). The region between these two lines is referred to as region I in the text. The real ζ axis and the two lines, $v^2 = 1 + 3u^2$, map to the imaginary σ axis. Each of these is shown with hatching on the side corresponding to $\mathrm{Re}(\sigma) < 0$ and an arrow pointing in the direction $\mathrm{Im}(\sigma) \to -\infty$ (see also Fig. 2). Light extended hatching shows the three regions which map to the lower half σ plane, $\mathrm{Im}(\sigma) < 0$.

contour for evaluating the density of states will be the real ζ axis.

IV. THE DENSITY OF STATES

As was mentioned in Sec. I, with the usual definition of the partition function in statistical mechanics, the number density of states of a system with energy E in an interval dE can be computed by the inverse Fourier-Laplace transform (1.2) of the partition function. The resolution of the square root introduced in the previous section to make the action and the inverse temperatures single valued, and the choice of contour we discussed there, ensure that this integral for $\nu(E)$ becomes regular for all finite energies, real or complex. We now investigate some pertinent properties of $\nu(E)$, looking at the semiclassical regime $r_0 \gg r_p$ in which a saddle-point approximation is applicable.

By defining a shifted dimensionless energy variable

$$\eta = \frac{GE}{r_0} - 1 , \tag{4.1}$$

and a dimensionless large parameter

$$\lambda = \frac{4\pi r_0^2}{r_p^2} , \tag{4.2}$$

we can write the density of states as

$$\nu(\eta, r_0) \approx \frac{2r_0}{\hbar} \int_{-\infty}^{\infty} d\zeta (1 + 3\zeta^2) \exp\{\lambda[-\tfrac{1}{4}(3\zeta^4 + 2\zeta^2 - 1) - i\eta\zeta(1+\zeta^2)]\} . \tag{4.3}$$

To obtain a saddle-point approximation to the integral, we distort the original contour until it becomes (in this case) a path of steepest descent passing through a saddle point of the exponent. Our path originates at $\zeta = -\infty$, passes through a stationary (maximum) point at some $\zeta = \zeta_0$ which lies on the imaginary axis, then proceeds symmetrically to $\zeta = +\infty$. For η real and $|\eta| < 3^{-1/2}$ we find $\zeta_0 = -i\eta$, while for $|\eta| > 3^{-1/2}$ we have $\zeta_0 = -i3^{-1/2}\mathrm{sgn}(\eta)$.

Just as for the partition function (1.1), a zero-order approximation to the integral (4.3) is given by the value of the integrand at the saddle point of the exponent [cf. (1.3)]. A more refined approximation includes contributions from the dominant part of the exponent in the vicinity of the saddle point. Except when η satisfies

$$\left| |\eta| - \frac{1}{\sqrt{3}} \right| \le O(\lambda^{-1/3}) , \tag{4.4}$$

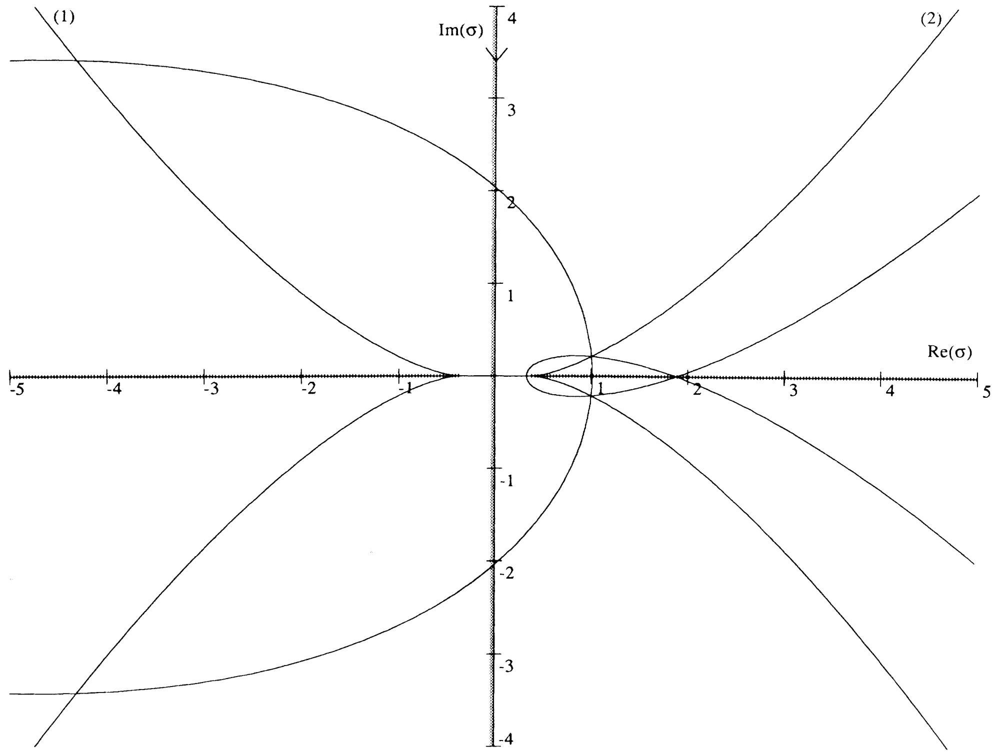

FIG. 2. One sheet for the complex σ variable: namely, that corresponding to region I (see text), the central region of the complex ζ plane referred to in Fig. 1. This middle sheet has two cuts along the real axis, from $2(27)^{-1/2}$ to $+\infty$ and from $-2(27)^{-1/2}$ to $-\infty$, the other two sheets each having only one of these cuts. The imaginary axis has the $\mathrm{Re}(\sigma)<0$ side hatched and an arrow pointing in the direction $\mathrm{Im}(\sigma)\to-\infty$ (see also Fig. 1). The two lines labeled (1) and (2) are the images of the straight lines $\mathrm{Im}(\zeta)=\pm(3)^{-1/2}$ similarly labeled in Fig. 1. The images of two other lines, $\mathrm{Im}(\zeta)=1.3(3)^{-1/2}$ and $-2.3(3)^{-1/2}$, are also shown. Along with line (2) they all pass through the point $\sigma\sim1.004+0.2136i$, though each is on a different sheet.

the dominant term in the exponent in (4.3) is quadratic, and we obtain

$$\nu(\eta,r_0)\sim\frac{r_p}{\hbar}[2(1-3\eta^2)]^{1/2}\exp\left[\frac{\lambda}{4}(1-\eta^2)^2\right],\qquad \frac{1}{\sqrt{3}}-|\eta|>O(\lambda^{-1/3}), \tag{4.5}$$

and

$$\nu(\eta,r_0)\sim\frac{3r_p}{\hbar\lambda}(\sqrt{3}|\eta|-1)^{-5/2}\times\exp\left[\frac{\lambda}{3\sqrt{3}}(\sqrt{3}-2|\eta|)\right],\qquad |\eta|-\frac{1}{\sqrt{3}}>O(\lambda^{-1/3}). \tag{4.6}$$

Precisely at $|\eta|=3^{-1/2}$, the dominant term is cubic, giving

$$\nu(\eta,r_0)\sim\frac{2r_p\sqrt{\pi}}{\hbar\Gamma(\frac{1}{3})}\left[\frac{2}{\sqrt{3}\lambda}\right]^{1/3}\exp\left[\frac{\lambda}{9}\right]. \tag{4.7}$$

By including the contribution from both the quadratic and the cubic dependence of the exponent in the vicinity of the saddle point, we can obtain for *all* real η an approximation in terms of Airy functions,[9,10] which always captures the leading behavior of the integral, even when (4.4) holds, while passing smoothly between approximations (4.5) and (4.6). This approximation is given by

$$\nu(\eta,r_0)=\frac{2r_0}{\hbar}\left[(1+3\zeta_0^2)-2i\zeta_0\frac{a_2}{a_3}-\frac{2a_2^2}{3a_3^2}\right]I_0-\frac{2r_0}{\hbar}\left[6i\zeta_0+\frac{2a_2}{a_3}\right]I_1, \tag{4.8}$$

where

$$I_0=\exp\left[\lambda\left[a_0+\frac{2a_2^3}{27a_3^2}\right]\right]\frac{2\pi}{|3a_3\lambda|^{1/3}}\times\mathrm{Ai}\left[\frac{a_2^2\lambda^{2/3}}{|3a_3|^{4/3}}\right], \tag{4.9}$$

$$I_1=\exp\left[\lambda\left[a_0+\frac{2a_2^3}{27a_3^2}\right]\right]\frac{2\pi\,\mathrm{sgn}(a_3)}{|3a_3\lambda|^{2/3}}\times\mathrm{Ai}'\left[\frac{a_2^2\lambda^{2/3}}{|3a_3|^{4/3}}\right], \tag{4.10}$$

$$a_0=-\tfrac{3}{4}\zeta_0^4-\tfrac{1}{2}\zeta_0^2-i\eta_0(1+\zeta_0^2)+\tfrac{1}{4}\ , \tag{4.11}$$

$$a_2=\tfrac{9}{2}\zeta_0^2+\tfrac{1}{2}+3i\eta\zeta_0\geq 0\ , \tag{4.12}$$

$$a_3=3i\zeta_0-\eta\ , \tag{4.13}$$

and ζ_0 is as given above. In the Appendix we give infinite-series expressions for $\nu(\eta,r_0)$ which are convergent everywhere, but are of practical significance only in a number of isolated domains of η. The approximations (4.5) and (4.6) are asymptotic to the respective leading terms of these series, all of which, when (4.4) holds, fail to be useful, whereas (4.8) remains valid.

As described in Sec. II, the expectation value of the energy in a box of radius r_0 and inverse temperature $\beta=4\pi r_0\sigma$ can be computed from its definition (2.8). Letting

$$\sigma=-i\zeta_H(1+\zeta_H^2)\ , \tag{4.14}$$

we have in terms of our new energy variable

$$\langle\eta(r_0,\beta)\rangle=\langle\eta(r_0,\zeta_H)\rangle=\eta_0\ , \tag{4.15}$$

where

$$-\frac{1}{\sqrt{3}}\leq\eta_0=i\zeta_H=-\left[1-\frac{r_+}{r_0}\right]^{1/2}\leq 0\ . \tag{4.16}$$

This determines the "physical" range of η in accordance with (2.12). The exponent of $\nu(\eta,r_0)$ evaluated at the mean energy is

$$\frac{\pi r_0^2}{r_p^2}(1-\eta_0^2)^2=\frac{\pi r_+^2}{r_p^2}\ . \tag{4.17}$$

This result is the entropy (2.9) of the stable black hole, as indeed it should be semiclassically. Outside the physical range, for large positive η, we see from (4.6) that $\nu(\eta,r_0)$ is exponentially decreasing, which is more than adequate for the partition function to be well defined and make physical sense. We also see in (4.6) that for large negative η, $\nu(\eta,r_0)$ is again (linearly) exponentially decreasing, a point relevant to our discussion of the complete inversion of the above calculation in the next section. There we obtain exactly $Z_0(r_0,\zeta)$ by a Fourier-Laplace transform of the exact $\nu(\eta,r_0)$ given by (4.3). For the present, we content ourselves with a saddle-point evaluation of Z_0 by using our saddle-point approximation (4.5) for $\nu(\eta,r_0)$ in the range $|\eta|\leq 3^{-1/2}$, which includes the entire physical range. We find

$$\begin{aligned}Z&\sim\frac{r_0}{r_p^2}\int_{-1/\sqrt{3}}^{1/\sqrt{3}}d\eta\,\nu(\eta,r_0)\exp[-\lambda(\eta+1)\sigma]\\&\sim\exp\{\lambda[-\tfrac{1}{4}(3\eta_0^4-2\eta_0^2-1)+i\zeta_H(1+\zeta_H^2)]\}\ ,\end{aligned} \tag{4.18}$$

with

$$\frac{1}{\sqrt{3}}+i\zeta_H>O(\lambda^{-1/3})\ . \tag{4.19}$$

and $\eta_0=i\zeta_H$ is the saddle point along the path of integration. A comparison of (4.18) with (3.3) substituted in (1.3) demonstrates that we have obtained precisely Z_0. Thus, our adopted-definition and interpretation of ν are consistent.

V. AN INTEGRAL TRANSFORM DERIVED FROM ITS INVERSE

To determine the precise way in which the partition function $Z_0(r,\zeta_H)$ can be given in terms of our computed $\nu(\eta,r_0)$, we go back to the definition (4.3) of ν as an integral and try to establish an identity between Z_0 and the Fourier-Laplace transform of ν. For ζ_H corresponding to a stable black hole ($0<-i\zeta_H<3^{-1/2}$), consider

$$\begin{aligned}Z_\epsilon(r_0,\zeta_H)&=\frac{r_0}{G}\int_{-1}^{\epsilon\infty}d\eta\,\nu(\eta,r_0)\exp[-\lambda(\eta+1)\sigma]\\&=2\left[\frac{r_0}{r_p}\right]^2\int_{-1}^{\epsilon\infty}d\eta\,e^{-\lambda\sigma}\int_{-\infty}^{\infty}d\zeta(1+\zeta^2)\exp(\lambda\{-\tfrac{1}{4}(3\zeta^4+2\zeta^2-1)-\eta[\sigma+i\zeta(1+\zeta^2)]\})\ ,\end{aligned} \tag{5.1}$$

where $\epsilon=\pm 1$. Z_+ corresponds to the usual Laplace transform of ν. For ζ varying along the real axis and for σ corresponding to ζ_H in the physical domain, we have

$$\mathrm{Re}[\sigma+i\zeta(1+\zeta^2)]>0\ , \tag{5.2}$$

and the order of integration can be interchanged in Z_+ [similarly for ζ varying along the line $\mathrm{Im}(\zeta)=-3^{-1/2}$]. Alternatively, for ζ varying along the line $\mathrm{Im}(\zeta)=3^{-1/2}$, which is also a valid distortion of the contour for obtaining $\nu(\eta,r_0)$, we have

$$\mathrm{Re}[\sigma+i\zeta(1+\zeta^2)]<0\ , \tag{5.3}$$

and the order of integration can only be interchanged for Z_-. An example using a particular value of ζ_H is shown in Fig. 3. We then have

$$Z_\epsilon=\frac{1}{2\pi i}\int_{-\infty-i\epsilon 1/\sqrt{3}}^{\infty-i\epsilon 1/\sqrt{3}}d\zeta\left[\frac{1+3\zeta^2}{-i\sigma+\zeta(1+\zeta^2)}\right]\exp\{\lambda[-\tfrac{1}{4}(3\zeta^4+2\zeta^2-1)+i\zeta(1+\zeta^2)]\}\ . \tag{5.4}$$

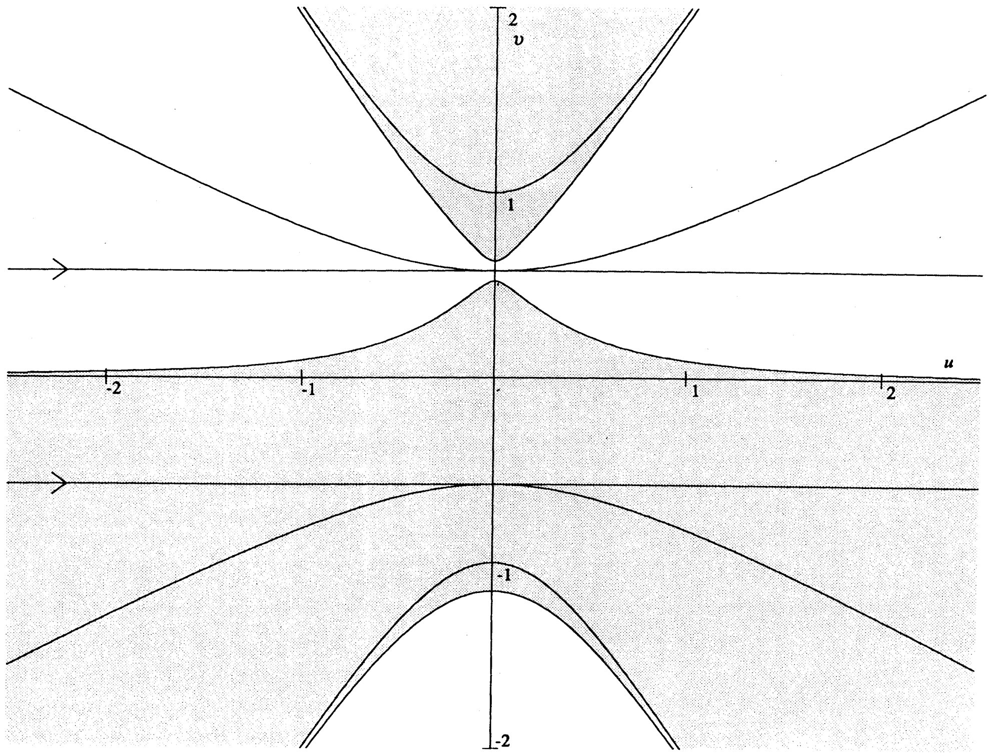

FIG. 3. The complex ζ plane ($\zeta = u + iv$). For the particular value $\zeta_H = 0.9i(3)^{-1/2}$, $\sigma = 1.971(27)^{-1/2}$, the order of integration of ζ and η can be inverted for Z_+ in the shaded region, and in the unshaded region it can be inverted for Z_- (see text). On the boundary both inversions are possible; the η integration for Z_0 becomes a δ function and the ζ integration is then immediate. For $\sigma > 2(27)^{-1/2}$ neither of the boundary curves above the real axis cut the imaginary axis [they pinch off around $\zeta_H = i(3)^{-1/2}$] so inversion of the order of integration becomes impossible.

We have introduced Z_- because numerical work showed us that we can never expect Z_+ and Z_0 to be identical, and Z_- shows us how to correct for the difference. In the double integral (5.1) for Z_-, we were free to move the path of integration from $\mathrm{Im}(\zeta)=0$ to $\mathrm{Im}(\zeta)=3^{-1/2}$ without changing the result. However, in moving the contour in the single-integral expression (5.4), we see that we pick up a contribution from the residue of the isolated single pole of the integrand at $\zeta = \zeta_H$; the other poles do not contribute. This residue is exactly Z_0, which we are seeking, as it should be. Thus we have

$$Z_0 = Z_+ - Z_- = \frac{r_0}{G} \int_{-\infty}^{\infty} d\eta\, \nu(\eta, r_0) \exp[-\lambda(\eta+1)\sigma] , \tag{5.5}$$

with $0 < -i\zeta_H < 3^{-1/2}$. We have found unambiguously the transform, by the inverse of which ν had originally been calculated. We refer to Z_0 and ν as being related by a Fourier-Laplace transform (5.5) and its inverse (4.3). Once we have this result, we can see how to derive it more directly by changing the order of integration along the line $\mathrm{Re}[\sigma + i\zeta(1+\zeta^2)] = 0$ and obtaining from the η integral a δ function: $\delta(\zeta(1+\zeta^2) - i\sigma)$.

The method we have used gives more than we have obtained so far. With the contour for Z_+ moved to the line $\mathrm{Im}(\zeta) = -3^{-1/2}$, we see that our result actually holds for the extended domain

$$-\frac{1}{\sqrt{3}} < i\zeta_H < \frac{1}{\sqrt{3}} . \tag{5.6}$$

By a careful analysis of the integrand, and by using the principal value for integrals when the pole lies on a contour, we can also show that our result applies at the end points $-i\zeta_H = \pm 3^{-1/2}$. Furthermore, by considering all those complex values of ζ_H to which our method is applicable, we find that our result holds in the entire strip

$$|\sigma| \le \frac{2}{3\sqrt{3}} . \tag{5.7}$$

We now turn to examine the contribution of the negative energy tail, that is, of Z_-, to the total partition function. Thus, consider

$$Z_0{}^{-1} \frac{r_0}{G} \int_{-\infty}^{-\eta_c} d\eta\, \nu(\eta, r_0) \exp[-\lambda(\eta+1)\sigma] . \tag{5.8}$$

When

$$\eta_c - \frac{1}{\sqrt{3}} > O(\lambda^{-1/3}) , \tag{5.9}$$

this is approximated by

$$\sim Z_0^{-1}(3^{1/4}2\sqrt{\pi}\sqrt{\lambda})^{-1}\int_{\eta_c}^{\infty} d\,|\eta|\,(|\eta|-3^{-1/2})^{-5/2}\exp\left\{\lambda\left[\tfrac{1}{3}-\sigma-|\eta|\left[\frac{2}{3\sqrt{3}}-\sigma\right]\right]\right\}, \tag{5.10}$$

$$=Z_0^{-1}(48\pi^2\lambda^2)^{-1/4}\exp\left\{\lambda\left[\tfrac{1}{9}-\sigma\left[1-\frac{1}{\sqrt{3}}\right]\right]\right\}\{(\tfrac{2}{3}\Delta^{-3/2}-\tfrac{4}{3}\lambda\delta\Delta^{-1/2})\exp(-\lambda\delta\Delta)+\tfrac{4}{3}(\pi\delta^3\lambda^3)^{1/2}\mathrm{erfc}[(\lambda\delta\Delta)^{1/2}]\}\ , \tag{5.11}$$

where

$$\Delta=\eta_c-\frac{1}{\sqrt{3}},\quad \delta=\frac{2}{3\sqrt{3}}-\sigma\ . \tag{5.12}$$

The result (5.11) can be approximated as

$$\left[2\times 3^{1/4}\sqrt{\pi}\lambda^{3/2}\left[\eta_c-\frac{1}{\sqrt{3}}\right]^{5/2}\left[\frac{2}{3\sqrt{3}}-\sigma\right]\right]^{-1}\exp\left\{-\lambda\left[\frac{1}{\sqrt{3}}+i\zeta_H\right]^2\left[\frac{3}{4}\left[\frac{1}{\sqrt{3}}+i\zeta_H\right]\left[\frac{5}{3\sqrt{3}}-i\zeta_H\right]+\left[\eta_c-\frac{1}{\sqrt{3}}\right]\left[\frac{2}{\sqrt{3}}-i\zeta_H\right]\right]\right\}, \tag{5.13}$$

when

$$\frac{1}{\sqrt{3}}+i\zeta_H>O(\lambda^{-1/3})\ , \tag{5.14}$$

and as

$$\frac{1}{3^{5/4}\left[\pi\lambda\left[\eta_c-\frac{1}{\sqrt{3}}\right]^3\right]^{1/2}}\ , \tag{5.15}$$

when

$$\frac{1}{\sqrt{3}}+i\zeta_H\ll O(\lambda^{-1/3})\ . \tag{5.16}$$

From the definition of η, the contribution of the negative-energy tail is formed by taking $\eta_c=1$. It is exponentially small in (5.13). However, *at* $\zeta_H=i3^{-1/2}$, corresponding to the limiting temperature of a stable configuration, the exponential factor vanishes [see (5.15)] and the contribution is relatively large, that is, $O(r_p r_0^{-1})$. In a similar fashion, by changing the signs of ζ_H and σ everywhere in our result, but not that of η_c, we find that the contribution of the positive-energy tail, from $+\eta_c$ to $+\infty$, is also exponentially small except at $\zeta_H=-i3^{-1/2}$. Semiclassically, this behavior is entirely acceptable, although it is indicative of macroscopic quantum effects in the limit $|i\zeta_H|\to 3^{-1/2}$. A consequence of these effects can be seen by examining (2.10); although energy fluctuations are typically of the order of the Planck mass, they receive a very large amplification as the limiting temperature for stability is approached.

VI. DISCUSSION

In the last four sections we have been considering black-hole thermodynamics, by which we mean thermodynamics based on stable classical black-hole solutions of the Einstein equation and derived as a zero-order approximation to a full quantum theory of gravitational thermodynamics for fields of black-hole topology $R^2\times S^2$. To discuss further black-hole thermodynamics in the wider context of gravitational thermodynamics, we select for particular attention three aspects of our results: (1) the exponential tails of $\nu(\eta,r_0)$ at large positive and negative energies; (2) the constraints on the range of σ for the existence of classical solutions; (3) the possibility for a discussion of negative temperature.

The need for all negative energies in the relation between a partition function and the underlying density of states is not uncommon in classical thermodynamics. A simple example arises when the binomial distribution of occupation numbers of a finite spin system is replaced by a Gaussian approximation which has tails to both $+\infty$ and $-\infty$. One is also familiar with a barrier, usually at $\beta=0$, restricting the domain of definition of a partition function. In black-hole thermodynamics, precisely because we have exponential decay for $\nu(\eta,r_0)$ at large positive and negative energies, we have only a strip for σ, marked by two barriers, neither of which is at zero. This is in contrast with the original constraint (2.6) which was concerned only with real positive σ in this strip. With the extension to negative σ provided by (5.7), discussion of negative temperatures becomes possible. Negative temperatures are hotter and have greater positive mean energies than occurs for *any* positive temperature.[11,12] In black-hole thermodynamics, negative temperatures arise on the second sheet, corresponding to $\mathrm{Re}(\zeta)<0$, of the square root in a red-shift factor for β in (2.4). These states are in accord with the constraint (2.13) because of the double-valued dependence of $r_+r_0^{-1}$ on ζ.

The possibility of discussing negative temperatures is a demonstrable property of the single-valued action (3.3), although it was not a property of the original derivation of Z_0 from classical solutions. On the other hand, the original constraint on σ in (2.6) was introduced through the dependence on stable classical solutions, but would not be expected to apply in a full quantum theory. The linear exponential tails in ν are intimately related to the constraints (5.7) placed on σ and we shall argue below that these tails would *not* be an essential feature of the full theory. However, we already know from (4.18) that some energies outside the "physical" range (2.12) are certainly necessary in black-hole thermodynamics in order to establish even an approximate relation between Z_0 and ν. This additional range of energies corresponds exactly to the range of mean energies for allowable systems at negative temperature. Thus, negative temperature arises in a natural and consistent way for the single-valued action of black-hole thermodynamics, although our treatment does not indicate how a state of the gravitational field at negative temperature should be prepared. In any event, the usefulness of our result will also depend on how a black hole at negative temperature could be brought into thermal contact with a system that may include matter at positive temperature.

We remarked in the Introduction that Z_0 is not a Laplace transform. This is because, unlike a Laplace transform, Z_0 is bounded for $|\mathrm{Re}(\sigma)| \le 2(27)^{-1/2}$ but not in a right half-plane $\mathrm{Re}(\sigma) > \sigma_0$ for any σ_0. We shall now show that two aspects of black-hole thermodynamics which we have mentioned above are consequences of this: namely, (1) the exponential tails of $\nu(\eta, r_0)$ and (2) the restriction $|\mathrm{Re}(\sigma)| \le 2(27)^{-1/2}$. These consequences are not peculiar to gravity. In order to understand better the general context in which they arise, we consider two simple examples. We imagine that these examples result from reducing some path integral to an integration over a single degree of freedom, leading to an effective action for the remaining variable. Because we propose no specific physical models for the examples, we take all variables to be dimensionless.

Let us first consider an effective action

$$I_{\mathrm{eff}} = \gamma^2 x^2 - 2x(\beta - \beta_0) , \tag{6.1}$$

and define the partition function

$$Z(\beta_0) = \int_0^\infty dx \, \exp[-I_{\mathrm{eff}}(\beta, x)] . \tag{6.2}$$

An exact evaluation of the partition function yields

$$Z(\beta) = \frac{\sqrt{\pi}}{2\gamma} \{\exp[\gamma^{-2}(\beta_0 - \beta)^2]\} \mathrm{erfc}[-\gamma^{-1}(\beta_0 - \beta)] . \tag{6.3}$$

The density of states

$$\nu(E) = \frac{1}{2\pi i} \int_{-i\infty + c}^{i\infty + c} d\beta \, Z(\beta) \exp(\beta E) \tag{6.4}$$

is most easily computed by using (6.2) and changing the order of integration. We find

$$\nu(E) = \tfrac{1}{2} \exp(-\tfrac{1}{4}\gamma^2 E^2 + \beta_0 E) , \tag{6.5}$$

from which we can reconstruct the partition function by the usual Laplace integral

$$\begin{aligned} Z(\beta) &= \int_0^\infty dE \, \nu(E) \exp(-\beta E) \\ &= \int_0^\infty dx \, \exp[-\gamma^2 x^2 + 2x(\beta_0 - \beta)] . \end{aligned} \tag{6.6}$$

Alternatively, we could have started with the zero-loop approximation. The effective action has a single stationary point at

$$x_0 = \gamma^{-2}(\beta_0 - \beta) , \tag{6.7}$$

which is always a global minimum for the action. However, this point lies in the domain of definition of x only if

$$\beta < \beta_0 . \tag{6.8}$$

Therefore, we have a restriction on the range of β for which the approximation

$$Z_0 = \exp[\gamma^{-2}(\beta_0 - \beta)^2] \tag{6.9}$$

is valid. As in our discussion of the black hole, Z_0 is not a Laplace transform. Nevertheless, the inversion integral is well defined. We obtain

$$\nu_0(E) = \frac{\gamma}{2\sqrt{\pi}} \exp(-\tfrac{1}{4}\gamma^2 E^2 + \beta_0 E) , \tag{6.10}$$

which differs from the exact result only by a constant factor. However, to construct Z_0 from ν_0, we must integrate over the whole energy range $(-\infty, \infty)$, which gives

$$Z_0(\beta) = \int_{-\infty}^\infty dE \, \nu_0(E) \exp(-\beta E) , \tag{6.11}$$

as can be most readily seen by the method we used in the previous section. Although β was restricted so that we could obtain the zero-loop approximation (6.9), relation (6.11) can be used in the entire complex β plane as the relation (6.7) between β and x_0 is single valued. In this particular example, we can easily perform a "one-loop" approximation, by which we mean, expand the effective action through quadratic order around x_0 and then use a saddle-point approximation to the integral. We obtain

$$Z_1(\beta) = \frac{\sqrt{\pi}}{\gamma} \exp[\gamma^{-2}(\beta_0 - \beta)^2] , \tag{6.12}$$

whose inversion would lead to the exact expression (6.5) for $\nu(E)$, but a Fourier-Laplace integral is still required to recover Z_1 from it.

In our second example we take

$$I_{\mathrm{eff}} = \tfrac{1}{3}\gamma^2 x^3 - x(\beta - \beta_0) , \tag{6.13}$$

from which we can obtain the exact partition function as in (6.2). From this we can evaluate the density of states as in the previous example to find

$$\nu(E) = \exp(-\tfrac{1}{3}\gamma^2 E^3 + \beta_0 E) , \tag{6.14}$$

which again leads back to the original partition function by a Laplace transform as in (6.6). Alternatively, for the zero-loop approximation, we begin by noting that the effective action has two stationary points

$$x_0 = \pm \frac{1}{\gamma} (\beta_0 - \beta)^{1/2} . \tag{6.15}$$

These occur at real x_0 only if $\beta < \beta_0$ as in the previous example. In this case, the positive stationary point is always a minimum of the action and we obtain

$$Z_0(\beta)=\exp\left[\frac{2}{3\gamma}(\beta_0-\beta)^{3/2}\right], \tag{6.16}$$

which cannot be a Laplace transform. Here, the partition function does not become single valued until we introduce the uniformizing variable

$$\zeta=-(\beta_0-\beta)^{1/2}. \tag{6.17}$$

The complex β plane must be cut along the positive real axis from β_0 to ∞, which corresponds to the entire imaginary axis for ζ. As in the case of the black hole, we choose the β sheet associated with the thermodynamically stable classical solution—here, the minimum point of the action—which is equivalent to requiring $\mathrm{Re}(\zeta)<0$. We then obtain

$$\begin{aligned}\nu_0(E)=2\left[\frac{\gamma}{2}\right]^{2/3}\left\{E\left[\frac{\gamma}{2}\right]^{2/3}\mathrm{Ai}\left[E^2\left[\frac{\gamma}{2}\right]^{4/3}\right]\right.&\\ \left.-\mathrm{Ai}'\left[E^2\left[\frac{\gamma}{2}\right]^{4/3}\right]\right\}&\\ \times\exp(-\tfrac{1}{6}\gamma^2E^3+\beta_0E)\,.&\end{aligned} \tag{6.18}$$

For large γ we can obtain the leading behaviors to be compared, respectively, with (4.5), (4.6), and (4.7):

$$\nu_0(E)\sim\frac{\gamma E^{1/2}}{\sqrt{\pi}}\exp(-\tfrac{1}{6}\gamma^2E^3+\beta_0E),\quad E>O(\gamma^{-2/3})\,, \tag{6.19}$$

$$\nu_0(E)\sim(4\sqrt{\pi}\gamma\,|\,E\,|^{5/2})^{-1}\exp(\beta_0E),\quad -E>O(\gamma^{-2/3})\,, \tag{6.20}$$

$$\nu_0(E)\sim\frac{2^{4/3}\gamma^{2/3}}{3^{1/3}\Gamma(\frac{1}{3})},\quad E=0\,. \tag{6.21}$$

These expressions correspond to saddle-point approximations to $\nu_0(E)$ in each case. As before, a Fourier-Laplace transform (6.11) is required to reconstruct Z_0, but now this is possible only when $\beta<\beta_0$.

From the second example, we see that a critical point in the uniformizing transformation leads to linear exponential tails in $\nu_0(E)$. This indicates that part of the range of E is not to be included in the Laplace transform for the exact partition function. Similarly, we see that the restriction on β is another artifact of the approximation. It does not apply to the exact results.

From these observations we can draw some conclusions about our study of the black hole. First, although $\nu(\eta,r_0)$ has linear exponential tails for $|\eta|\gg 3^{-1/2}$, these are consequences of the zero-loop approximation. Thus we deduce that the energy in *gravitational* thermodynamics in the black-hole topological sector is actually bounded above and below; however, our first example indicates that the information we have used so far is insufficient for us to decide where the exact bounds lie. Second, although *black-hole* thermodynamics requires for its existence a restriction on the boundary data β and r_0, this restriction does not apply to the path integral definition of the partition function of gravitational thermodynamics in the relevant topological sector. The zero-loop approximation, depending for its validity on the existence of stable classical solutions, has introduced this constraint.

VII. CONCLUSION

In the development of black-hole thermodynamics, the introduction of a finite radius for the system turned out to be a very important refinement, as was the corresponding realization that thermodynamic stability occurs only for the larger black hole whenever the boundary data β and r_0 indeed permit any such classical solution. With an infinite box only the unstable black hole has a finite mass, and this fact has been a source of difficulty in earlier discussions. When classical stability allows a black hole to occupy a finite box, black-hole thermodynamics exists, in every essential way equivalent to any classical thermodynamical theory. Contrary to previous belief, there is, in fact, a well-defined canonical ensemble. We have used its partition function to obtain a similarly well-defined density of states for the corresponding microcanonical ensemble. From this, we have argued that for quantum-gravitational thermodynamics in the black-hole topological sector, energy will be bounded from above and below. The restriction on σ required for the existence of stable classical solutions does not apply to the exact partition function as defined by a path integral over all relevant metrics. Our treatment would seem to be entirely in accord with classical thermodynamics and its derivation from quantum-statistical mechanics.

We have found that negative temperature arises in a natural and consistent way once the action for black-hole thermodynamics has been made single valued. Possible physical implications of this must await further study.

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APPENDIX: EXACT EXPRESSIONS FOR THE DENSITY OF STATES $\nu(\eta,r_0)$

We shall obtain exact expansions for $\nu(\eta,r_0)$ by computing higher terms in the saddle-point approximation in a particular way. We start with the contour chosen as a straight line passing through the saddle point, which gives

$$\begin{aligned}\nu(\eta,r_0)=\frac{2r_0}{\hbar}\int_{-\infty}^{\infty}d\zeta(1+3\zeta_0^2+6\zeta_0\zeta+3\zeta^2)&\\ \times\exp[\lambda(a_0-a_2\zeta^2+ia_3\zeta^3-\tfrac{3}{4}\zeta^4)]\,,&\end{aligned} \tag{A1}$$

where λ,a_0,a_2,a_3 are defined in (4.2) and (4.11)–(4.13) and ζ_0 is the saddle point:

$$\zeta_0 = -i\eta \quad \text{for } |\eta| < \frac{1}{\sqrt{3}} ,$$
$$\zeta_0 = -\frac{i\eta}{\sqrt{3}\,|\eta|} \quad \text{for } |\eta| > \frac{1}{\sqrt{3}} . \tag{A2}$$

We evaluate the integral exactly by expanding the exponential of the cubic term as a power series and using the relation

$$\int_{-\infty}^{\infty} d\zeta\, \zeta^{2p} \exp(-y\zeta^2 - \tfrac{1}{2}\zeta^4) = 2\Gamma(p+\tfrac{1}{2}) D_{-(p+1/2)}(y) \exp(y^2/4), \quad p \in Z , \tag{A3}$$

where D is a parabolic cylinder function.[13,14]

For $|\eta| < 3^{-1/2}$ we can substitute for ζ_0 in the coefficients and integrate by parts to obtain

$$v(\eta, r_0) = -\frac{2r_0}{\hbar\lambda} \int_{-\infty}^{\infty} \frac{d\zeta}{\zeta^2} \exp[\lambda(a_0 - a_2\zeta^2 + ia_3\zeta^3 - \tfrac{3}{4}\zeta^4)] . \tag{A4}$$

Since only even terms in the expansion will contribute to the integral, we find a single sum:

$$v(\eta, r_0) = -\frac{3r_0}{\hbar} \left[\frac{2}{3\lambda}\right]^{3/4} \exp\left[\lambda\left[a_0 + \frac{a_2^2}{6}\right]\right] \times \sum_{m=0}^{\infty} (-1)^m \frac{\Gamma(3m - \frac{1}{2})}{(2m)!} [(\tfrac{2}{3})^{3/2} \lambda^{1/2} a_3^2]^m \times D_{1/2-3m}\left[a_2 \left[\frac{2\lambda}{3}\right]^{1/2}\right] . \tag{A5}$$

When (4.5) is valid, it is given by the leading behavior of the first term in this series. Only the first term survives for $a_3 = 0$, and this gives the exact result at $\eta = 0$:

$$v(0, r_0) = \frac{r_p}{\hbar} \sqrt{2} \left[\frac{6}{\lambda}\right]^{1/4} \exp\left[\frac{7\lambda}{24}\right] D_{1/2}\left[\left[\frac{\lambda}{6}\right]^{1/2}\right] . \tag{A6}$$

Although the series is convergent, successive early terms all become comparable for $a_2^3 \leq O(\lambda^{-1})$, which corresponds to the condition (4.4), and the sum is no longer useful.

For $|\eta| > 3^{-1/2}$, we have $1 + 3\zeta_0^2 = 0$, and we can again integrate by parts to obtain

$$v(\eta, r_0) = -\frac{2ir_0}{a_3\hbar} \int_{-\infty}^{\infty} d\zeta (4\zeta + 3\zeta^3) \exp[\lambda(a_0 - a_2\zeta^2 + ia_3\zeta^3 - \tfrac{3}{4}\zeta^4)] . \tag{A7}$$

Now only odd terms from the expansion of the cubic term in the exponent will contribute to the integral, and there is a separate series for each term in the coefficient of the exponential, giving

$$\begin{aligned} v(\eta, r_0) = &-\frac{12r_0}{\hbar a_3^2} \left[\frac{2}{3\lambda}\right]^{3/4} \exp\left[\lambda\left[a_0 + \frac{a_2^2}{6}\right]\right] \\ &\times \sum_{m=1}^{\infty} \frac{(-1)^m \Gamma(3m - \frac{1}{2})}{(2m-1)!} [(\tfrac{2}{3})^{3/2} \lambda^{1/2} a_3^2]^m D_{1/2-3m}\left[a_2\left[\frac{2\lambda}{3}\right]^{1/2}\right] \\ &- \frac{6r_0}{\hbar a_3^2 \lambda} \left[\frac{2}{3\lambda}\right]^{1/4} \exp\left[\lambda\left[a_0 + \frac{a_2^2}{6}\right]\right] \sum_{m=1}^{\infty} \frac{(-1)^m \Gamma(3m + \frac{1}{2})}{(2m-1)!} [(\tfrac{2}{3})^{3/2} \lambda^{1/2} a_3^2]^m D_{-1/2-3m}\left[a_2\left[\frac{2\lambda}{3}\right]^{1/2}\right] . \end{aligned} \tag{A8}$$

When (4.6) is valid the dominant behavior comes from the first term in the first series, of which (4.6) is the leading approximation. For $a_3 = 0$ only the first term in each series survives and we obtain an exact result at $|\eta| = \sqrt{3}$ which, by use of the recurrence relation [see (A10)] for $D_{-q}(y)$, becomes

$$v(\sqrt{3}, r_0) = \frac{r_p}{\hbar\lambda} \frac{3}{2^{5/2}} \left[\frac{8\lambda}{3}\right]^{3/4} \times \exp\left[\frac{\lambda}{3}\right] D_{-3/2}\left[\left[\frac{8\lambda}{3}\right]^{1/2}\right] . \tag{A9}$$

The result (A8) is again not useful for $a_2^3 \leq O(\lambda^{-1})$, but for a_2 exactly zero, i.e., $|\eta| = 3^{-1/2}$, it is identical with (A5) term by term as a power series in λ, as can be seen by further use of the recurrence relation:

$$yD_{-q}(y) - D_{-q+1}(y) + qD_{-q-1}(y) = 0 . \tag{A10}$$

The relation of the approximations (4.5) and (4.6) to the leading behavior in the series (A5) and (A8) can be established by the use of the asymptotic result

$$D_{-q}(y) \sim y^{-q} \exp(-\tfrac{1}{4}y^2), \quad q \ll y \to \infty , \tag{A11}$$

whereas convergence of the series depends on

$$D_{-q}(y) \sim \frac{\sqrt{\pi}\, 2^{-q/2}}{\Gamma(\frac{1}{2}(1+q))} \exp[-y(q - \tfrac{1}{2})^{1/2}] , \quad y^2 \ll q \to \infty . \tag{A12}$$

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