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NEW HORIZONS IN THERMODYNAMICS

BY

GEOFFREY GORDON HAYWARD

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To whom it may concern:

I hereby agree to let Geoffrey Gordon Hayward include the paper entitled "*Primordial black holes in the very early Universe*" coauthored by him and myself as part of his thesis.

Sincerely,

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The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research for acceptance, a thesis entitled "New Horizons in Thermodynamics" submitted by Geoffrey Gordon Hayward in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Theoretical Physics.

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To Mom and Dad

Abstract

This thesis collects five papers which treat the theory of horizon thermodynamics and its applications to cosmology.

In the first paper I consider general, spherically symmetric spacetimes with cosmological and black hole horizons. I find that a state of thermal equilibrium may exist in classical manifolds with two horizons so long as a matter distribution is present. I calculate the Euclidean action for non–classical manifolds with and without boundary and relate it to the grand canonical weighting factor. I find that the mean thermal energy of the cosmological horizon is negative.

In the second paper I derive the first law of thermodynamics for bounded, static, spherically symmetric spacetimes which include a matter distribution and either a black hole or cosmological horizon. I calculate heat capacities associated with matter/horizon systems and find that they may be positive or negative depending on the matter configuration. I discuss the case in which the cosmological constant is allowed to vary and conclude that the Hawking/Coleman mechanisms for explaining the low value of the cosmological constant are not well formulated.

In the third paper, co–authored by Jorma Louko, we analyze variational principles for non-smooth metrics. These principles give insight to the problem of constructing minisuperspace path integrals in horizon statistical mechanics and quantum cosmology. We demonstrate that smoothness conditions can be derived from the variational principle as equations of motion. We suggest a new prescription for minisuperspace path integrals on the manifold $\bar{D} \times S^2$.

In the fourth paper, I examine the contribution of the horizon energy density to black hole temperature. I show the existence of positive heat capacity solutions in the small mass regime.

In the fifth paper, co-authored by Diego Pavón we investigate the role of primordial black holes in the very early universe under $SU(3) \times SU(2) \times U(1)$, $SU(5)$, and their supersymmetric counterparts. Three of the four theories predict a phase in which black holes and radiation are of comparable energy density. The fourth theory, $SU(5)$, predicts a radiation dominated model from the Planck era onward.

In the concluding general discussion I show how generalized laws of thermodynamics can be related to variations of the classical gravitational action. These laws apply even for non-static, non-spherically symmetric spacetimes.

Preface

The University of Alberta Faculty of Graduate Studies and Research currently accepts two styles of thesis: the 'traditional format' and the 'paper format'. I have prepared this thesis in the paper format. In it, I present five separate studies on the theory of horizon thermodynamics and its cosmological implications. The first three address fundamental theoretical issues while the last two apply the theory to problems which arise in cosmology.

This progression from theory to application harmonizes well with the ideal of scientific inquest. But, in fact, for me, the progression has been in exactly the opposite direction: from applied theory back to the basics.

The last two papers in the thesis were actually written first; in the summer and fall of 1988[1]. At this time, I assumed that the theory of horizon thermodynamics and statistical mechanics was generally well understood. I made standard assumptions in applying the theory to problems of black hole dynamics. I have since learned, however, that the theory of horizon thermodynamics can be very subtle and is not generally well understood.

As I became aware of the perils of simplistic assumptions about the thermodynamic properties of horizons, I became increasingly interested in basic theoretical issues. The first three papers collected in this thesis address some of these issues[2].

With my research, into basic horizon thermodynamics, my understanding

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[1] G. Hayward, "*Black holes with positive specific heat*", Class. Quantum Grav. 6 (1989) L25; G. Hayward and D. Pavón, "*Black holes in the very early Universe*", Phys. Rev. D 40 (1989) 1748.

[2] G. Hayward, "*Euclidean action and the thermodynamics of manifolds without boundary*", Phys. Rev. D 41 (1990) 3248.
G. Hayward, "*The first law and horizon thermodynamics*", to appear in Phys. Rev. D.
G. Hayward and J. Louko, "*Variational principles for non-smooth metrics*", to appear in Phys. Rev. D.

of the subject has evolved enormously. While this is encouraging for me, it has some negative consequences for the reader. There is an abrupt change between the formalism and theoretical assumptions employed in the first three papers and those employed in the last two. After I have invested so much energy developing a particular theoretical approach to the thermodynamics of horizon/matter systems in the first three papers, the reader could be forgiven for wondering why I adopt a much more simplistic approach in the last two. The reason for the shift is simply that in the two years since the last two papers were written, much has changed both in my understanding of horizon thermodynamics and in the discipline itself.

Yet, despite the simplicity of certain assumptions made in the analysis of the last two papers, I believe that the findings presented there are interesting and, for the most part, essentially correct. Severe limitations to our observational powers in the Universe introduce many uncertainties into the numerical analysis of the final paper. Nonetheless, I believe it is very important to at least attempt to come to terms with the real world in which we actually live. The last two papers are written in this spirit.

In addition to the introduction and the five central papers, I present a concluding chapter of general discussion. This final chapter is much more than a summary of the five preceding papers. In it, I make important generalizations of the findings reported in the body of the thesis and derive a number of new and provocative results. I believe the results of this last chapter have important implications not just for the treatment of horizons in cosmology but for our understanding of thermodynamics itself.

Acknowledgements

I am very much indebted to Werner Israel. When I came to the University of Alberta, he immediately welcomed me as a Ph. D. student even though I had at that time no knowledge of general relativity, tensor analysis or even differential geometry. Through the last four years, he has provided me with guidance and encouragement. Always, he has been willing to listen and to set me straight when I go astray. His excellence in both teaching and research are an inspiration to me.

I am also indebted to Jim York for a series of discussions we had on a week-end in the Fall of 1989. In these discussions, he explained his approach to black hole thermodynamics. These discussions were both stimulating and inspirational. While an enormous amount of work has been done on horizon thermodynamics, I believe the approach to horizon thermodynamics initiated by Jim York allows for a profundity and consistency of analysis not matched by the more traditional methods. The York method is the launching point for most of the analysis of this thesis.

I am grateful to Diego Pavón for many valuable discussions. It was he who aroused my interest in the thermodynamics of cosmological horizons. The work of Chapter 6 was co-authored by him.

I am very grateful to Jorma Louko for the many insights he has afforded me. The work presented in Chapter 4 was co-authored by him.

I am also grateful to Don Page for providing invaluable comments on various manuscripts and for numerous energetic discussions on horizon thermodynamics.

Discussions with Hans Kunzle, Des McManus, and Jason Twamley have given me valuable insight into problems discussed in this thesis.

Above all, I am grateful to my wife Denyse. Only she knows all the support she has given through all stages of preparation of this thesis. Her faith in me through the many set backs I have encountered has made this thesis possible.

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CHAPTER 1

INTRODUCTION

1.1 Overview

It was a tremendous shock to the physics community when Hawking [1] discovered that event horizons, such as that of a black hole, emit radiation. Before Hawking's discovery, the horizon of a black hole was thought to be a one way surface: objects could fall in, but nothing, not even light could escape out. At a classical level, this picture is perfectly correct. However, Hawking found that when one incorporates the effects of quantum theory, particles are able to tunnel back across the event horizon.

Yet, even more stunning than the discovery that horizons emit radiation, was the fact that this radiation has an exactly thermal spectrum. This fact immediately confirmed Bekenstein's insightful speculations on a connection between black hole entropy and surface area [2]. It was now clear that a point had been divined at which three streams of physical thought—thermodynamics, general relativity and quantum field theory—all converge.

Aptly, the expression relating a horizon's temperature, T, to its surface gravity, $\kappa(G)$,

$$T = \frac{\hbar\kappa(G)}{2\pi kc}, \qquad (1.1.1)$$

involves all four of the fundamental constants of nature. It is tempting to imagine that this formula, as enigmatic in its simplicity as $F = Ma$ or $E = Mc^2$, yet distilling information from three widely disparate fields of physics, may prove something of a Rosetta stone as we try to decode the mystery of quantum gravity. At very least, Hawking's formula for horizon temperature has become the cornerstone for a theory of horizon thermodynamics.

By now, a solid core of work has been done on the thermodynamic properties of horizons. Many of the peculiar twists that they afford, like negative heat capacities and the ambiguity of the vacuum state, have now been mastered. Increasingly, efforts are turning toward the task of incorporating the effects of horizons in a generalized theory of thermodynamics. We are tantalizing close to realizing this goal.

In recent years, work has begun to develop a general theory of quantum gravitational statistical mechanics using horizon thermodynamics as a guide. Notably, a paper by Whiting and York [3] gives some intriguing insight into how to evaluate the grand canonical partition function associated with a black hole in a box. This field of research is particularly interesting because of the profound connections between gravitational statistical mechanics and the path integral approach to quantum gravity [4].

Other potentially interesting applications of horizon thermodynamics are to problems in semi-classical cosmology. For instance, many models of the Universe involve a period of inflationary expansion. Such inflationary expansion can lead to the formation of a cosmological event horizon. Yet very little is known about how the thermodynamic properties of such an event horizon might influence the evolution of the Universe. Also, it is probable that quantum gravitational tunneling in the very early Universe led to a copious production of mini-black holes, yet it has not been clear how the thermodynamic properties of these black holes could influence the subsequent evolution of the Universe.

This thesis collects five papers concerned with developing the theory of horizon thermodynamics and with applying it to problems in classical and quantum cosmology. In this introduction, I lay some essential groundwork for the papers which follow. Section 2 reviews a derivation of the Hawking temperature for vacuum, static, spherically symmetric spacetimes. Section 3 generalizes this derivation to allow for the presence of a matter distribution. Section 4 focuses on the special case in which the horizon is a cosmological horizon. Section 5 considers the connections between the Euclidean action of a system and its free energy with special attention to the role played by boundary conditions. Section 6 reviews the thermodynamics of a Schwarzschild black hole in a box held at constant temperature and surface area. Finally, Section 7 is a synopsis of the thesis.

1.2 The different faces of horizon temperature

The beauty of the Hawking temperature result is that it connects seemingly unrelated branches of physics. A less attractive consequence is that it is often necessary to understand the result at several different levels. Depending on circumstances, it may be valuable to interpret Hawking radiation in the context of quantum field theory, thermal field dynamics, differential topology, or even classical thermodynamics.

In Appendix A, I sketch the derivation provided by Hartle and Hawking [5] which obtains the Hawking temperature result in a quantum field theoretic setting. Appendix B reviews the Israel derivation [6] in which the result appears in the context of thermal field dynamics.

In this section, I show how a topological constraint gives rise to horizon thermal radiation at the Hawking temperature. The program is as follows. One demands that the Euclidean sector associated with a spacetime be regular. For vacuum spacetimes with horizons, this uniquely fixes the period of the proper

Euclidean time variable. All continuous functions of the metric components—in particular, the Feynman propagator—will then be periodic in the Euclidean sector with this fixed period. Meanwhile, a thermal state is characterized by a Feynman propagator which is periodic in Euclidean time; the period being equal to the inverse temperature of the state. So, in essence, by fixing the periodicity of a metric in the Euclidean sector, a horizon fixes the temperature of the state described by that metric.

First, focus on static spherically symmetric vacuum solutions to Einstein's equations. In the Euclidean sector, these metrics have the form[1],

$$ds^2 = f(r)\,d\tau^2 + f(r)^{-1}\,dr^2 + r^2 d\Omega^2. \tag{1.2.1}$$

where τ is periodic but with undetermined period and $G = c = k = \hbar = 1$. Further suppose that $f(r_+) = 0$ and $f > 0$ for $r > r_+$. Then the 2-surface $r = r_+$ may be interpreted as a black hole outer event horizon.

The Euclidean sector extends over $r \geq r_+$. For a generic choice of the periodicity of the Euclidean time coordinate τ, a metric of the form (1.2.1) has an intrinsic singularity at $r = r_+$. The behavior of the metric in the limit of approach to the singularity is clear after making the coordinate transformation

$$R = \frac{2f(r)^{1/2}}{f'(r_+)}, \tag{1.2.2}$$

where a prime indicates partial differentiation with respect to r. Metric (1.2.1) becomes

$$\left(\frac{f'(r_+)}{2}\right)^2 R^2\,d\tau^2 + \left(\frac{f'(r)}{f'(r_+)}\right)^2 dR^2 + r^2\,d\Omega^2. \tag{1.2.3}$$

[1]The lapse function, $g_{00}^{1/2}$, of metrics solving Einstein's equations is only specified up to an arbitrary constant. The convention of Hartle and Hawking [5] and Israel [6] is to absorb this arbitrariness into the periodicity of the Euclidean time coordinate τ and set $g_{00} \to 1$ as $r \to \infty$. The constraint that the metric be regular in the Euclidean sector then fixes the periodicity of the coordinate τ. I adopt this convention for the purposes of this section, but will adopt a different convention in sections which follow.

Note that the metric component $g_{RR} \rightarrow 1$ as $r \rightarrow r_+$. If the metric is not to have a conical singularity at the black hole horizon, we require that the coordinate τ have a period $\frac{4\pi}{f'(r_+)}$.

Now return to the original form of the metric (1.2.1). The condition that the Euclidean sector be regular, constrains the otherwise arbitrary period of the Euclidean time coordinate τ. The local period in proper Euclidean time for an observer at radial coordinate r is then

$$\frac{4\pi f(r)^{1/2}}{f'(r_+).} \tag{1.2.4}$$

Since, the metric has a local period in proper Euclidean time given by expression (1.2.4), functions of metric such as the Feynman propagator must also have a proper Euclidean time periodicity given by this expression. Furthermore, the local period of the Feynman propagator in proper Euclidean time is equal to its inverse temperature. A schematic demonstration of this is given by Wald [7]. I now review this argument.

Recall that the density matrix for a quantum mechanical system in a thermal equilibrium state at inverse temperature β is just

$$\rho = \frac{e^{-\beta H}}{\mathrm{Tr}\,\{e^{-\beta H}\}}, \tag{1.2.5}$$

where H is the Hamiltonian of the system and β is the inverse temperature of the system. Furthermore, in the Heisenberg representation, the time evolution of observables $\hat{O}$ is given by

$$\hat{O}(t + t_0) = e^{iHt}O(t_0)e^{-iHt}. \tag{1.2.6}$$

While it is not possible to define rigorously a Hamiltonian operator in quantum field theory, equations (1.2.5) and (1.2.6) still apply in a formal sense even for quantum fields. Hence, apply (1.2.6) to a Klein–Gordon scalar field $\phi(x)$ to get

$$\phi(\vec{x}, t + i\beta) = e^{-\beta H}\phi(\vec{x}, t)e^{\beta H}. \tag{1.2.7}$$

Recall that the Wightman function for the scalar field is defined by

$$W(x_1, t_1|x_2, t_2) \equiv Z^{-1}\langle \mathrm{Tr} e^{-\beta H}\phi(x_1, t_1)\phi(x_2, t_2)\rangle, \tag{1.2.8}$$

where $Z \equiv \mathrm{Tr}\ \{e^{-\beta H}\}$. Then use the cyclical property of the trace and (1.2.7) to determine that

$$\begin{aligned} W(x_1, t_1|x_2, t_2) &= Z^{-1}\langle \mathrm{Tr} e^{-\beta H}\phi(x_1, t_1)e^{\beta H}e^{-\beta H}\phi(x_2, t_2)\rangle \\ &= W(x_2, t_2|x_1, t_1 + i\beta) \\ &= W(x_2, t_2 - i\beta|x_1, t_1). \end{aligned} \tag{1.2.9}$$

Now consider the thermal Feynman propagator analytically continued to the Euclidean sector with $\tau = -it$;

$$G_F(x_1, \tau_1|x_2, \tau_2) = W(x_1, \tau_1|x_2, \tau_2)\theta(\tau_1 - \tau_2) + W(x_2, \tau_2|x_1, \tau_1)\theta(\tau_2 - \tau_1). \tag{1.2.10}$$

Appeal to (1.2.9) with, for instance, $\tau_1 < \tau_2 < \beta$, to obtain that

$$G_F(x_1, \tau_1|x_2, \tau_2) = G_F(x_1, \tau_1 + \beta|x_2, \tau_2). \tag{1.2.11}$$

Thus, the thermal propagator is periodic in Euclidean time with period equal to the inverse temperature of the system.

Combining the above result with the fact that the presence of a regular horizon imposes a proper Euclidean time periodicity given by (1.2.4), one has that the local horizon temperature at r is given by

$$T(r) = \frac{f'(r_+)}{4\pi}f(r)^{-1/2}. \tag{1.2.12}$$

To compare this expression with the Hawking formula, we require an expression for the surface gravity, κ, of a black hole horizon. The surface gravity of a horizon is defined by

$$\xi^a \nabla_a \xi^b \Big|_{r=r_+} \equiv \xi^b \Big|_{r=r_+} \kappa, \tag{1.2.13}$$

where ξ^a is the future directed timelike Killing field which agrees with the null geodesic generator on the black hole future horizon.

To obtain an expression for κ, convert to advanced Eddington–Finkelstein coordinates,

$$ds^2 = -f(r)\, dv^2 + 2\, dv\, dr + r^2\, d\Omega^2, \tag{1.2.14}$$

where $v = t + r_*$ is advanced time and r_* is the Regge–Wheeler tortoise coordinate defined (up to an irrelevant additive constant) by the integral,

$$r_* = \int^r f(r)^{-1}\, dr. \tag{1.2.15}$$

Projecting onto the v, r subspace,

$$\xi^a = [1, 0]\,. \tag{1.2.16}$$

while the null geodesic generator of the future horizon is

$$l^a = \left[1, \frac{1}{2} f(r)\right], \tag{1.2.17}$$

A straightforward calculation yields

$$\kappa = \frac{1}{2} f'(r)\Big|_{r_+}. \tag{1.2.18}$$

Now compare expression (1.2.18) for the surface gravity of the black hole with expression (1.2.12) for the local temperature at r to obtain

$$T(r) = \frac{\kappa}{2\pi} f(r)^{-1/2}. \tag{1.2.19}$$

This is just the Hawking expression corrected for the local 'Tolman factor' $f(r)^{-1/2}$.

Note that due to the presence of the Tolman factor, the temperature is not uniform throughout the manifold. The Hawking temperature quoted in equation (1.1.1) is actually the horizon temperature as measured by an observer at infinity where $f = 1$. Since $f(r) \to 0$ as one approaches to the horizon, the local temperature measured in the vicinity of the horizon approaches infinity.

To see why this should be, consider the fact that when an observer accelerates, he measures a thermal bath of particles at a temperature directly related to his acceleration [8]. As one approaches the horizon, the local gravitational force on an observer diverges. This force is equal and opposite to the force required to keep a static observer from falling into the black hole. Hence, with respect to free falling observers, a static observer near the horizon undergoes enormous acceleration. It is this effective local acceleration which causes him to observe a bath of thermal particles at enormous temperature.

1.3 The effects of matter

An important limitation to the derivation of horizon temperature provided above is that it does not account for the 'backreaction' of particle fields on the geometry. The very fact that particle–antiparticle pairs are produced in the region outside the black hole undercuts our initial assumption that the region outside the black hole satisfies $G_{\mu\nu} = 0$ and so can be described by a metric of the form (1.2.1). The backreaction problem has been examined by a number of authors (for instance, [9,10,11]). I examine some thermodynamic consequences of backreaction effects in Chapter 5.

While the backreaction problem *per se* does not concern us here, it is clear that any self consistent treatment of black hole thermodynamics must allow for the presence of a matter distribution in the region outside the horizon. Now extend the above analysis to this more general case.

The spherically symmetric static solution to the Euclidean Einstein's equations for an uncharged black hole surrounded by a matter distribution with energy density $\rho(r)$ and radial pressure $p(r)$ is

$$ds^2 = e^{2\psi(r)} f(r)\, d\tau^2 + f(r)^{-1}\, dr^2 + r^2\, d\Omega^2, \tag{1.3.1}$$

where

$$\begin{aligned} f(r) &= 1 - \frac{r_+}{r} - \frac{\int_{r_+}^{r} 8\pi \rho r^2\, dr}{r} \\ \frac{\partial \psi}{\partial r} &= 4\pi(\rho + p) r V(r)^{-1}. \end{aligned} \tag{1.3.2}$$

As in the vacuum case, $f(r_+) = 0$ and $f(r) > 0$ for $r > r_+$ where the r_+ is the horizon radius. Also, in keeping with the conventions of the previous section, we normalize so that $g_{00} \to 1$ as $r \to \infty$ and note that the period of the Euclidean time parameter τ is to be determined by the condition that the metric be regular at the horizon.

As in the vacuum case, make use of the coordinate transformation $R = 2f(r)^{1/2}/f'(r_+)$. Regularity of the metric at the horizon requires that the period of the Euclidean time coordinate τ be

$$\frac{4\pi e^{-\psi(r_+)}}{f'(r_+)}. \tag{1.3.3}$$

To calculate the surface gravity of the horizon, express metric (1.3.1) in advanced Eddington–Finkelstein coordinates,

$$ds^2 = -e^{2\psi(r)} f(r)\, dv^2 + e^{\psi(r)}\, dv\, dr + r^2\, d\Omega, \tag{1.3.4}$$

where $v = t + r_*$ is advanced time and r_* is the Regge–Wheeler coordinate given up to a constant (which we may take to be zero) by,

$$r_* = \int^r e^{-\psi(r)} f(r)^{-1}\, dr. \tag{1.3.5}$$

Let ξ^a be the future directed Killing field which matches the null geodesic generator on the black hole future horizon. Note that the v, r projection of ξ^a is

$$\xi^a = [1, 0]\,, \tag{1.3.6}$$

while the null geodesic generator of the future horizon is

$$l^a = \left[1, \frac{1}{2} e^{\psi(r)} f(r)\right]. \tag{1.3.7}$$

so by virtue of the definition of surface gravity (1.2.13),

$$\kappa = \frac{1}{2} e^{\psi(r)} f'(r)\Big|_{r=r_+}. \tag{1.3.8}$$

Now use expression (1.3.3) for the period of τ, metric (1.3.1), expression (1.3.8) for the surface gravity, and the fact that inverse temperature is equal to the period of proper Euclidean time to obtain

$$T(r) = \frac{e^{\psi(r_+)-\psi(r)} f'(r_+)}{4\pi} f(r)^{-1/2} = \frac{\kappa}{2\pi} g_{00}^{-1/2}. \tag{1.3.9}$$

This is the expression for the local Hawking temperature at r of the horizon when a matter distribution is present. [For the case in which the matter distribution outside the black hole approximates Page's stress tensor, this result was obtained by York [9].]

Note that in the presence of a matter distribution, the Euclidean topological constraint does not in itself uniquely specify the temperature throughout the spacetime. The local temperature at r, through its dependence on $\psi(r)$ and $f(r)$

depends implicitly on the matter configuration between r_+ and r. For matter distributions everywhere satisfying the condition $\rho + p > 0$, the effect of the matter distribution is to lower the temperature measured at r. Physically, the reason for this is that the radiation coming from the black hole suffers a greater gravitational redshift due to the presence of the matter between the horizon and the observer.

1.4 Hawking temperature for cosmological horizons

For cases in which the spacetime has a cosmological horizon rather than a black hole horizon, the treatment is only slightly different. Nonetheless, confusion over the sign of both the Hawking temperature and the surface gravity can easily arise. It is valuable, therefore, to review the treatment for cosmological horizons explicitly.

Assume a static, spherically symmetric matter distribution and that a cosmological horizon occurs at r_{++}. Also, for simplicity, restrict attention to the case in which no black hole horizon occurs so that the Euclidean sector extends from $r = 0$ to $r = r_{++}$. The solution to the Euclidean Einstein equations has the form of (1.3.1) where $f(r)$ and $\psi(r)$ are given by

$$\begin{aligned} f(r) &= 1 - \frac{r_{++}}{r} - \frac{\int_{r_{++}}^{r} 8\pi\rho r^2\,dr}{r} \\ \frac{\partial\psi}{\partial r} &= 4\pi(\rho + p)r\,f(r)^{-1}. \end{aligned} \tag{1.4.1}$$

Now impose the regularity condition at the horizon to find that the period of the Euclidean time parameter τ is

$$-\frac{4\pi e^{-\psi(r_{++})}}{f'(r_{++})}. \tag{1.4.2}$$

The negative sign appears because $f'(r_{++})$ is negative definite and the quantity of interest is actually the absolute value of the period. [For instance, integrals over

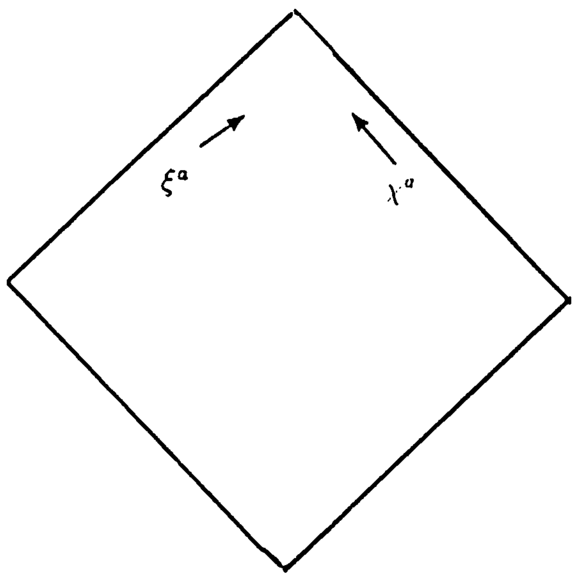

Figure 1.1: Kruskal diagram for a static, spherically symmetric spacetime with black hole and cosmological horizons. Here, ξ^a is the future directed Killing field which agrees with the null geodesic generator on the black hole future horizon and χ^a is the future directed Killing field which agrees with the null geodesic generator on the cosmological future horizon.

Euclidean time in the four dimensional action proceed from $\tau = 0$ to $\tau = \tau_f$ where τ_f is the (positive) period of τ.]

Now calculate the horizon's surface gravity. Note that the generator of the future cosmological horizon is not covered by advanced Eddington-Finkelstein coordinates [12] (see Figure 1.1). To obtain the surface gravity of the cosmological horizon, resort to the retarded Eddington–Finkelstein metric,

$$ds^2 = -e^{2\psi(r)} f(r)\, du^2 - 2e^{\psi(r)}\, du\, dr + r^2\, d\Omega^2, \qquad (1.4.3)$$

where $u = t - r_*$ is retarded time and $r_* = \int^r e^{-\psi(r)} f(r)^{-1}\, dr$. Now let χ^a be the future directed Killing field which agrees with the null geodesic generator on the future cosmological horizon. The components of χ^a in the u, r plane are

$$\chi^a = [1, 0] \tag{1.4.4}$$

while the null generator has components,

$$m^a = \left[1, -\frac{1}{2} e^{\psi(r)} f(r)\right]. \tag{1.4.5}$$

The surface gravity of the cosmological horizon is then defined by

$$\chi^a \nabla_a \chi^b \Big|_{r=r_{++}} \equiv \chi^b \Big|_{r=r_{++}} \kappa, \tag{1.4.6}$$

which quickly yields

$$\kappa = -\frac{1}{2} e^{\psi(r)} \frac{\partial f(r)}{\partial r}\Big|_{r=r_{++}}. \tag{1.4.7}$$

Use equation (1.4.7) for the surface gravity, expression (1.4.2) for the periodicity of τ, metric (1.3.1), and the relation between the local period of Euclidean proper time and inverse temperature to find that

$$T(r) = -\frac{e^{\psi(r_{++}) - \psi(r)} f'(r_{++})}{4\pi} f(r)^{-1/2} = \frac{\kappa}{2\pi} g_{00}^{-1/2}. \tag{1.4.8}$$

This is the Hawking expression for the local temperature of a cosmological horizon at r. Both temperature and surface gravity are positive.

Note that as in the case of a black hole horizon, when a matter distribution is present, the temperature measured due to a cosmological horizon depends on the matter configuration between the observer and the horizon. So long as $\rho + p > 0$, the effect of this matter distribution is to *increase* the measured temperature of the cosmological horizon. In essence, the matter gravitationally blueshifts the radiation coming from the horizon.

Having reviewed the central features of the Hawking temperature associated with static, spherically spacetimes, I now move on to consider the connection between the Euclidean action of a spacetime and its free energy. By exploiting this connection, it is ultimately possible to derive all thermodynamic properties of a spacetime.

1.5 Euclidean action and free energy

Much of the progress that has been made in recent years in the study of horizon thermodynamics makes use of a fundamental connection between the classical Euclidean action of a manifold and its grand canonical free energy. This connection arises essentially due to a formal equivalence between the Euclideanized quantum gravitational path integral and the grand canonical partition function for a gravitating system [13]

Consider the case of a scalar field $\phi(x)$ defined on a manifold $\mathcal{M}$. The probability amplitude for the field to go from a configuration ϕ_1 at t_1 to a configuration ϕ_2 at t_2 is given by

$$\langle\phi_2, t_2|\phi_1, t_1\rangle = \langle\phi_2|e^{-iH(t_2-t_1)}|\phi_1\rangle, \tag{1.5.1}$$

where H is a time independent Hamiltonian. By breaking the time interval $t_2 - t_1$ up into infinitesimal intervals δt, this amplitude may be expressed as a path integral over all paths starting at the configuration ϕ_1 at t_1 and ending at configuration ϕ_2 at t_2,

$$\langle\phi_2, t_2|\phi_1, t_1\rangle = \int \delta\left[\phi\right] e^{iI_{\mathrm{L}}[\phi]}, \tag{1.5.2}$$

where $I_{\mathrm{L}}[\phi]$ is a Lorentzian action of the form

$$I_{\mathrm{L}}[\phi] = \int_{t_1}^{t_2} \mathcal{L}_{\mathrm{L}}\, d^3x\, dt, \tag{1.5.3}$$

with $\mathcal{L}_{\mathrm{L}}$ being the appropriate Lagrangian density.

If one sets $\phi_2 = \phi_1$ and $t_2 = t_1 + i\beta$ and rotates to the Euclidean sector so that $\tau = it$, one has from (1.5.1) and (1.5.2) that

$$\mathrm{Tr}\ e^{-\beta H} = \int \delta\left[\phi\right] e^{-I_{\mathrm{E}}[\phi]}, \tag{1.5.4}$$

where

$$I_{\mathrm{E}}[\phi] = \int_0^\beta \mathcal{L}_{\mathrm{E}}\, d^3x\, d\tau, \tag{1.5.5}$$

The left hand side of (1.5.4) is just the canonical partition function, Z. The right hand side is just the Euclidean path integral over all paths extending over all fields with period β in Euclidean time.

When conserved particle quantities such as charge or particle number are allowed to vary freely, the appropriate partition function is that of the grand-canonical ensemble and equation (1.5.4) becomes

$$Z = \mathrm{Tr}\ e^{-\beta(H-\mu_i N_i)} = \int \delta\left[\phi\right] e^{-I_{\mathrm{E}}[\phi]}, \tag{1.5.6}$$

where the μ_i are the (fixed) chemical potentials associated with the N_i and a summation over i is implied.

As noted by Gibbons and Hawking [13], the dominant contribution to the path integral should come from the classical trajectories. When the gravitational field is included in the path integral, this means that the path integral should be dominated by the action I_0 associated with the classical metric solution g_0 and the classical field solution ϕ_0. Expressing the metric and scalar field respectively by

$$\begin{aligned} g &= g_0 + \tilde{g} \\ \phi &= \phi_0 + \tilde{\phi}, \end{aligned} \tag{1.5.7}$$

Perform a Volterra functional expansion of the action around its classical value,

$$I = I_0 + I_2\left[\tilde{g}\right] + I_2\left[\tilde{\phi}\right] + \ldots. \tag{1.5.8}$$

Neglecting higher order terms,

$$\ln Z \simeq -I_0. \tag{1.5.9}$$

But, by definition, the free energy F is

$$F = E - TS - \mu_i N_i \equiv -\beta^{-1} \ln Z, \tag{1.5.10}$$

where E is the mean thermal energy of the system and S is its entropy. Hence, in the 'zero-loop' approximation,

$$I_0 = \beta F. \tag{1.5.11}$$

To make use of this connection between the classical action and the free energy, we require an expression for the gravitational action of a system. This turns out to be a more subtle problem than one might expect. Unlike the action functionals familiar from Newtonian mechanics, the gravitational action has terms with second order derivatives of the field variable. A consequence is that the appropriate gravitational action for a system depends on the boundary conditions imposed. This is a point of central importance.

For definiteness, consider a manifold $\mathcal{M}$ with a simply connected 3-boundary $\partial\mathcal{M}$. Represent the Euclidean 4-metric $g_{\mu\nu}$ (assumed C^2) in terms of the 3 + 1 ADM formalism. In this formalism, the line element is

$$ds^2 = \left(N^2 + N_i N^i\right) dr^2 + 2N_i dr dx^i + h_{ij} dx^i dx^j. \tag{1.5.12}$$

where N is the lapse, N^i is the shift vector and r is the ADM 'time' coordinate. Without loss of generality, let r range from 0 to 1. Identify the surface $r = 1$ with the boundary of the manifold. The surface $r = 0$ then corresponds to a locus in the interior of $\mathcal{M}$ and a coordinate singularity of the 3 + 1 metric representation.

The Euclidean Einstein–Hilbert gravitational action associated with the manifold is

$$I_{\mathrm{E.H.}} = -\frac{1}{16\pi}\int_{\mathcal{M}} R\, g^{1/2}\, d^4x. \tag{1.5.13}$$

Expressed in the ADM 3 + 1 formalism, this becomes

$$I = \int_{\mathcal{M}} \mathcal{L}\, d^4x + \frac{1}{8\pi}\int_{r=1} K\, h^{1/2}\, d^3x - \frac{1}{8\pi}\int_{r=0} K\, h^{1/2}\, d^3x, \tag{1.5.14}$$

where $\mathcal{L}$ is the first order Lagrangian scalar density,

$$\mathcal{L} = N\, h^{1/2}\left(K_{ij}K^{ij} - K^2 -{}^{(3)} R\right), \tag{1.5.15}$$

K_{ij} is the extrinsic curvature tensor associated with surfaces of constant r,

$$K_{ij} = \frac{1}{2N}\left(\frac{\partial}{\partial r}h_{ij} -{}^{(3)}\nabla_j N_i -{}^{(3)}\nabla_i N_j\right), \tag{1.5.16}$$

and where the final term in (1.5.14) is meant to be evaluated in the limit $r \rightarrow 0$.

Define momenta π^{ij} conjugate to h_{ij} by

$$\pi^{ij} \equiv \frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}}. \tag{1.5.17}$$

Obtain,

$$\pi^{ij} = \frac{1}{16\pi}\left(K^{ij} - h^{ij}K\right) h^{1/2}, \tag{1.5.18}$$

and, hence, the Hamiltonian formulation of the Einstein–Hilbert action (see Section 4.2),

$$I_{\mathrm{E.H.}} = \int_0^1 \left(\pi^{ij}\dot{h}_{ij} - N_i\mathcal{H}^i - N\mathcal{H}\right)\, d^3x\, dr - \int_1 \pi^{ij}h_{ij}\, d^3x + \int_0 \pi^{ij}h_{ij}\, d^3x. \tag{1.5.19}$$

Vary this action and integrate by parts to obtain (assuming smoothness at $r = 0$ which fixes the π^{ij} there),

$$\delta I_{\mathrm{E.H.}} = -\frac{1}{16\pi}\int_0^1 G_{\mu\nu}\, \delta g^{\mu\nu} g^{1/2}\, d^3x\, dr - \int_1 h_{ij}\, \delta\pi^{ij}\, d^3x. \tag{1.5.20}$$

To extremize the action under arbitrary variations $\delta g^{\mu\nu}$, each of the two terms above must independently go to zero. Setting the first term to zero under arbitrary variations gives the vacuum Einstein equations. However, whether or not the second term can be set to zero depends on what boundary conditions one attempts to impose.

If one attempts to fix the h_{ij} on the boundary to any non-trivial (ie. non-zero) values, the second term in (1.5.20) will not be zero for arbitrary variations $\delta\pi^{ij}$ and, hence, it will not be possible to extremize the action. On the other hand, if one fixes the π^{ij} on the boundary, the second term in (1.5.20) is automatically zero: extremization of the Einstein–Hilbert action with these boundary conditions, yields the ordinary Einstein equations.[2] One concludes that the Einstein–Hilbert action is appropriate if one wishes to fix the momenta π^{ij} on the boundary but not if one wishes to fix the intrinsic metric components h_{ij} there.

York [14] was the first to note that for the case in which one wishes to fix the intrinsic 3-metric components on the boundary, the appropriate action is

$$I_{\rm Y} = \frac{-1}{16\pi}\int_{\mathcal{M}} R\, g^{1/2}\, d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}} K\, h^{1/2}\, d^3x. \qquad (1.5.21)$$

Variation of the York action yields

$$\delta I_{\rm Y} = -\frac{1}{16\pi}\int_{\mathcal{M}} G_{\mu\nu}\,\delta g^{\mu\nu} g^{1/2}\, d^4x + \int_{\partial\mathcal{M}} \pi^{ij}\,\delta h_{ij}\, d^3x. \qquad (1.5.22)$$

Clearly, when h_{ij} is held fixed on the boundary, extremization of the York action yields the vacuum Einstein equations. On the other hand, the York action cannot be extremized under arbitrary variations if one attempts to hold the momenta π^{ij} fixed on the boundary.

[2] A third option would be to fix neither the h_{ij} nor the π^{ij} on the boundary. Since, both terms in (1.5.20) have to equal zero independently if the action is to be extremized, this option yields the ordinary Einstein equations, plus the 'surface Einstein equations' that $h_{ij} = 0$ on the boundary. The significance of these surface equations is considered in the context of the Kantowski-Sachs ansatz in Section 4.4

For thermodynamic applications it is often useful (though strictly unnecessary) to normalize the York action so that flat space has zero action. Including the appropriate normalization factor (first proposed by Gibbons and Hawking [13]), the corrected action becomes,

$$I_{\rm G.H.} = \frac{-1}{16\pi}\int_{\mathcal{M}} R\, g^{1/2}\, d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}} [K]\; h^{1/2}\, d^3x, \qquad (1.5.23)$$

where $[K] \equiv K - K_0$ and where K_0 is the trace of the extrinsic curvature of the boundary as measured in a flat 4–metric.

1.6 Schwarzschild black hole in the canonical ensemble

Armed with expression (1.5.11) relating the classical action to the free energy, and various alternative expressions for the gravitational action, now derive the thermodynamic properties of system consisting of a Schwarzschild black hole in a spherical 'box' held at fixed (inverse) temperature β_0 and surface area $4\pi r_0^2$. This problem was first examined by York [15]: many results which follow are due to him. However, the approach I use to derive these results differs in certain respects from York's. Notably, I do not put in the Hawking temperature as an assumption, but rather derive it as a result[3]

Of interest is the classical action associated with the manifold. Here, the word 'classical' implies imposing Einstein's equations for the vacuum, $G_{\mu\nu} = 0$ assuming static spherical symmetry. The metric solution to these equations with

[3] A different scheme for deriving the Hawking temperature from a 'reduced action' in which the Hamiltonian constraint and regularity at the horizon are imposed explicitly was devised by Whiting and York [3].

the proper length of the Euclidean time variable set to β_0 at r_0 is[4].

$$ds^2 = \left(\frac{\beta_0}{2\pi}\right)^2 \left(\frac{V(r)}{V(r_0)}\right) d\tau^2 + V(r)^{-1}\, dr^2 + r^2\, d\Omega^2, \qquad (1.6.1)$$

where τ has period 2π and $V(r) = \left(1 - \frac{r_+}{r}\right)$. While this metric satisfies Einstein's equations, it will, in general, have a conical singularity at the horizon.

Now, obtain an expression for the gravitational action appropriate to the given boundary conditions. To fix the temperature and surface area at the box is to fix the components of the intrinsic 3-metric there. Consequently, it is necessary to include the York boundary term in the gravitational action. To agree with standard conventions, one should also include the Gibbons–Hawking normalization factor. The manifold of interest has topology $\bar{D} \times S^2$ (here $\bar{D}$ indicates topology of a disc) and, in general, a conical singularity will contribute to the action (see Section 4.3). The contribution of the conical singularity is

$$I_{\text{c.s.}} = +\frac{1}{8\pi}\int_{r\to r_+} \left(K - \widehat{K}\right) h^{1/2}\, d^3x, \qquad (1.6.2)$$

where $\widehat{K}_{ij}$ is the extrinsic curvature associated with the three metric which has no conical singularity at the horizon. The gravitational action is then

$$\begin{aligned} I \;=\; & -\frac{1}{16\pi}\int_{\mathcal{M}} R\, g^{1/2}\, d^4x - \frac{1}{8\pi}\int_{r=r_0} [K]\; h^{1/2}\, d^3x \\ & +\frac{1}{8\pi}\int_{r\to r_+} \left(K - \widehat{K}\right) h^{1/2}\, d^3x. \end{aligned} \qquad (1.6.3)$$

Now calculate the classical action. The extrinsic curvature tensor is

$$K_{ij} = \frac{1}{2} V(r)^{1/2} \frac{\partial}{\partial r}\left(h_{ij}\right) \qquad (1.6.4)$$

where h_{ij} is the τ, θ, ϕ projection of metric (1.6.1). To obtain $K_{0\;ij}$, use (1.6.4) but substitute the fixed value $h_{\tau\tau}(r_0)$ for $h_{\tau\tau}(r)$. To obtain $\widehat{K}_{ij}$ use (1.6.4) but set

[4] Note this metric uses a different convention for normalizing g_{00} than that use in Sections 1.2, 1.3, and 1.4.

$h_{\tau\tau} = 4r_+^2 V(r)$. Also note, $R = 0$ for this system. Hence,

$$I = \beta_0 r_0 \left(1 - \left(1 - \frac{r_+}{r_0}\right)^{1/2}\right) - \pi r_+^2. \tag{1.6.5}$$

From the above and the relation between the classical action and the free energy, (1.5.11), obtain

$$F = r_0 \left(1 - \left(1 - \frac{r_+}{r_0}\right)^{1/2}\right) - \beta_0^{-1} \pi r_+^2. \tag{1.6.6}$$

Note that the free energy is a function of the fixed boundary data, β_0 and A_0, but also of the variable parameter r_+.

Extremize the free energy with respect to variations of r_+ to obtain the condition,

$$T_0 = \beta_0^{-1} = \frac{1}{4\pi r_+}\left(1 - \frac{r_+}{r_0}\right)^{-1/2}. \tag{1.6.7}$$

This is, of course, just the local Hawking temperature of the black hole as measured at the box. It is important to recognize the significance of this result.

All metrics of the form (1.6.1) are classical in the sense that they satisfy $G_{\mu\nu} = 0$ for $r_+ < r < r_0$ and the boundary conditions. They are, however, not necessarily classical from a thermodynamic perspective. In general, they have conical singularities at the horizon because, loosely speaking, the temperature of the black hole as measured at the box does not equal the temperature of the box as fixed by the external heat bath. However, the free energy of the system is extremized only for metrics which satisfy condition (1.6.7). This is precisely the condition that must be satisfied if no conical singularity is to occur at the horizon or, alternately, the condition that the box be in thermal equilibrium with the black hole.

The method used here differs from the standard treatment (see, for instance, [15,16,17]) which is to *assume* regularity at the horizon or, equivalently, the Hawking temperature relation[5]. Besides the shortcoming of assuming a central result which can otherwise be derived, the standard treatment suffers from a more serious ailment. To impose *a priori* regularity at the horizon may involve imposing constraints both on the intrinsic metric components and on their conjugate momenta there (see Section 4.3). Such a procedure is ill defined in the context of quantum theory.

Returning to the task of determining the thermodynamic properties of the black hole/box system, now consider (1.6.7) for the extremal values of r_+. If $r_0\beta_0^{-1} < \frac{\sqrt{27}}{8\pi}$ there are no positive real values of r_+ which satisfy (1.6.7) and, hence, no physically relevant extremal values for the free energy [15]. York concludes that black holes do not occur for such choices of boundary data. On the other hand, if $r_0\beta_0^{-1} > \frac{\sqrt{27}}{8\pi}$, there are two positive real solutions for r_+. The smaller black hole solution has $r_+ < 2r_0/3$, while for the larger solution $r_+ > 2r_0/3$.

Other thermodynamic properties are easy to derive. Make use of the classical thermodynamic relation

$$S \equiv \beta_0^2 \frac{\partial F}{\partial \beta_0}, \tag{1.6.8}$$

to obtain,

$$S = \pi r_+^2. \tag{1.6.9}$$

This , of course. is just the classic result that the entropy of a black hole is one fourth its horizon area. Similarly, note the relation between surface pressure, λ, and the free energy

$$\lambda \equiv -\frac{\partial F}{\partial A} \tag{1.6.10}$$

[5]In Ref. [15], York posits *ad hoc* equation (1.6.6) as a 'generalized free energy' in which r_+ is taken as a free variable and derives the Hawking temperature. A justification (different from the one offered above) for taking (1.6.6) as a generalized free energy is given by Whiting and York in Ref. [3].

gives a mean surface pressure at the box of

$$\sigma = -\left(1 - \left(1 - \frac{r_+}{r}\right)^{1/2} - \frac{r_+}{2r_0}\left(1 - \frac{r_+}{r}\right)^{-1/2}\right). \tag{1.6.11}$$

The mean thermal energy

$$E_0 = r_0\left(1 - \left(1 - \frac{r_+}{r}\right)^{1/2}\right) \tag{1.6.12}$$

obtains from the expression (1.6.6) and $F = E_0 - T_0 S$. and agrees with the energy one would expect on the basis of simple dynamical arguments [15]. The first law can then be expressed as

$$dE_0 = T_0\, dS - \sigma\, dA_0. \tag{1.6.13}$$

The heat capacity at fixed surface area is

$$C_A = \left(\frac{\partial E}{\partial T_0}\right)_A = 2\pi r_+^2 V(r_0)\left(\frac{3r_+}{2} - 1\right)^{-1}. \tag{1.6.14}$$

Note that for the smaller black hole solution the heat capacity is negative, whereas the larger black hole solution has positive heat capacity. One can also calculate a quantity analogous to the isothermal compressibility of the box [15];

$$\kappa_T(A) \equiv \frac{1}{A}\left[\frac{\partial A}{\partial \sigma}\right]_T. \tag{1.6.15}$$

Only for the larger black hole solution is this quantity positive. York concludes that only the larger black hole solution is locally stable.

1.7 Synopsis

The five papers to follow develop aspects of the theory of horizon thermodynamics and consider applications to problems which arise in semi-classical and quantum cosmology.

In the first paper, I consider systems which include a matter distribution and either a cosmological horizon or a black hole horizon or both. To my knowledge, this is the first treatment of a manifold with more than one horizon as a single thermodynamic system. Before this, it had not been clear how to define uniquely the temperature in a system with two horizons since each horizon dictates its own constraint on the temperature throughout the system.

I show that it is possible to define temperature uniquely throughout the system so long as a matter distribution is present and satisfies a general condition. I then calculate the Euclidean action for systems without boundary. I find that the action is equal to the the grand canonical weighting factor for a spacetime with zero mean thermal energy. Also, by calculating the Euclidean action for bounded spacetimes which include both a matter distribution and a cosmological horizon, I obtain an expression for the energy associated with a cosmological horizon. Remarkably, this energy proves to be negative.

In the second paper, I derive the generalized first law of thermodynamics for spherically symmetric static systems. This law applies to finite bounded systems which include both a matter distribution and either a black hole or a cosmological horizon. Several aspects of this law are new and interesting.

Most importantly, it bridges the gulf between horizon or 'topologically induced' thermodynamics on the one hand and classical 'statistically induced' thermodynamics on the other. It is the basis for a general theory of the thermodynamics of static, spherically symmetric systems including bot matter distributions and horizons. In contrast to a previous version of the first . .w for matter/black hole systems derived by Bardeen, Carter, and Hawking [18], the law I derive does not distinguish the thermodynamic properties of the horizon from those of the matter distribution. The law yields uniquely defined thermodynamic properties for the horizon/matter system as a whole.

Another important feature of the generalized first law is that it applies to systems with cosmological horizons. Beyond the fact that it is possible to associate a temperature and entropy with a cosmological horizon, there has been much confusion in the literature over how to treat the thermodynamics of systems with cosmological horizons. Much of this confusion can be traced directly to the absence of an expression for the first law associated with cosmological horizons. With the benefit of the first law, it is possible to define unambiguously the thermodynamic quantities relevant to such systems.

Another implication of the generalized first law is the well known result that the thermodynamic quantity conjugate to the cosmological constant is the four volume of the manifold (see, for instance, Ref.[19]). Consequently, if one wishes to choose an ensemble which allows for variation of the cosmological constant, one must constrain all members of the ensemble to have some fixed four volume. This fact has important implications for certain approaches to the problem of the low value of the cosmological constant. In particular, the Hawking/Coleman [20,21] mechanisms for explaining the low value of the cosmological constant are not well formulated.

Using the first law, I calculate heat capacities associated with various systems. I find that the heat capacity at fixed surface area of a black hole/matter system may be positive or negative depending on the matter configuration and on the boundary conditions imposed. Similarly, I find that the heat capacity associated with a system including a cosmological horizon and a matter distribution may be either positive or negative depending on the matter configuration and boundary conditions.

The third paper (co-authored by Jorma Louko) addresses an issue fundamental to the development of either a well defined theory of gravitational statistical mechanics or of quantum cosmology. The standard method [3,22,4] of gravitational statistical mechanics (or for that matter of quantum cosmology) is to employ a $3 + 1$ metric decomposition of the four-geometry of the manifold in question and then perform a mini–superspace path integral in terms of that decomposition. However, in many physically relevant manifolds it is valuable to choose a $3 + 1$ metric decomposition which does not completely cover the manifold but, rather, has a coordinate singularity at some fixed point set of a Killing vector field. For instance, in the manifolds with topology of a disc cross a 2–sphere discussed in the first two papers, it is valuable to choose a decomposition in which the fixed point set of the Killing field that transports around the disc appears as a coordiante singularity of the $3 + 1$ decomosition. At the level of the minisuperspace path integral, this coordinate singularity is the initial surface on which the metric field variables are to be defined. It is not at all clear what 'boundary conditions' should be imposed at this coordinate singularity.

The standard program [3,22,4] is to treat conditions which ensure smoothness at the coordinate singularity as 'boundary conditions' on the set of paths to be considered in the path integral. However, in general, there is not a one to one correspondence between smoothness conditions and independent metric fields which require boundary conditions. Simply to impose the smoothness conditions as boundary conditions results in constraining both a metric component and its conjugate momentum at the horizon which is clearly unacceptable in a quantum context. Furthermore, the dominant contribution to any path integral comes from paths which are not smooth [23]. Conditions which guarantee smoothness in a variational principle do not guarantee smoothness at the level of a path integral. Hence, the rationale for using such conditions as constraints on the paths to be included in the path integral is unclear.

We show that standard smoothness conditions imposed at the coordinate singularity may be relaxed while retaining a well defined variational principle. Variation of the Euclidean action with respect to non-smooth metrics then yields not only the standard Einstein equations but also regularity conditions at the coordinate singularity as equations of motion. This suggests the possibility of obtaining a well defined $3 + 1$ path integral formalism without imposing any 'boundary conditions' at the coordinate singularity. We sketch a path integral scheme which implements this idea. To actually evaluate the path integral using this scheme (or for that matter any $3 + 1$ path integral scheme), one would have to specify the appropriate contour of integration. We do not broach this issue in the paper.

The fourth paper in this thesis considers how back reaction effects in the Hartle–Hawking vacuum can lead to small mass black hole solutions with positive heat capacity. I show that if one incorporates contributions to the horizon temperature from vacuum polarization of the electromagnetic field, one can arrive at low temperature stable black hole configurations.

The fifth paper, co–authored by Diego Pavón, applies results of gravitational statistical mechanics and horizon thermodynamics to the problem of black hole formation in the very early Universe. Based on the probability of quantum gravitational tunneling from hot flat spacetime to Schwarzschild spacetime [24], and on the thermodynamic properties of black holes, it is possible to estimate black hole densities in the very early Universe.

In the paper we argue that three theories, the standard model, the supersymmetric standard model, and supersymmetric SU(5) all predict a 'binary phase' beginning at the Planck era in which black holes and ambient radiation are of comparable energy density. A fourth theory, SU(5), predicts a radiation dominated model from the Planck era onward. For those theories which predict a binary phase, the phase should last for a period between ten and a hundred Planck times. After this time the density of the black holes should drop off rapidly to a negligible fraction of the radiation energy density. We explore consequences related to baryogenesis, inflation theory, and the missing mass problem.

The final chapter of the thesis generalizes the results obtained in the five preceding studies. It is perhaps the most interesting chapter of the thesis. In it, I derive a general first law of thermodynamics which applies even to non-static, non-spherically symmetric systems. I extend the treatment to various ensembles other than the canonical and then to manifolds with non-connected boundaries or with no boundaries at all. I conclude the final chapter by obtaining generalized versions of the zeroth, second, and third laws of thermodynamics. In each case, the generalized laws relate to simple properties of the Euclidean action and its variations.

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CHAPTER 2

HERMODYNAMICS OF UNBOUNDED MANIFO]

In[1] recent years, important connections have been uncovered between the Euclidean action formulation of quantum gravity and what might be called the statistical mechanics of gravitational fields. The study of these connections has led to a deeper understanding of both quantum gravity and gravitational thermodynamics.

Gibbons and Hawking [1] were the first to point out the fundamental connections between the Euclidean action path integral and the partition function of the grand canonical ensemble. They examined four single horizon spacetimes—the Schwarzschild, Reissner–Nordström, Kerr and de Sitter. They argued that in each case the Euclidean gravitational action is equal to the inverse Hawking temperature times the grand canonical free energy. In other words, the path integral in the zero loop approximation is equal to the grand canonical partition function.

York [2] extended the work of Gibbons and Hawking to a black hole enclosed in a box at fixed temperature. York discovered that there are in fact two black hole solutions which satisfy the fixed temperature boundary condition. Whiting and York [3] broadly extended this work by examining general black hole topologies where the black hole is enclosed in a box of fixed temperature and G^0_0 is constrained to equal zero inside the box. They found that the 'reduced action' associated with these topologies is equal to the inverse temperature of the shell times the free energy of the black hole. Martinez and York [4] showed that this connection

[1] A version of this paper has been published:
G. Hayward, "Eucildean action and thermodynamics of manifolds without boundary," *Physical Review D* 41 (1990) 3248.

persists even if the box is filled with matter and that the entropy of the horizon and matter is additive.

In this paper, I calculate the Euclidean action for compact manifolds without boundary and explore its statistical mechanical significance. Specifically, I examine static, spherically symmetric spacetimes which have a cosmological horizon and possibly a black hole horizon. [In the Euclidean sector a horizon is not a boundary, rather it is constrained to be a regular 2-surface of the manifold[2].] First, I calculate the Euclidean action for these spacetimes without fixing the radial positions of the horizons or employing any fixed temperature shell. Then, I calculate the Euclidean action associated with the regions inside and outside a fixed temperature shell.

Consider a manifold $\mathcal{M}$ with the general static spherically symmetric Euclidean metric,

$$ds^2 = U(y)d\tau^2 + \frac{1}{V(y)}dy^2 + r^2(y)d\omega^2, \tag{2.1}$$

where τ is periodic with period 2π. Impose the following conditions on the manifold,

1. $U = \hat{V} = 0$ at $r = r_+$ and possibly at $r = r_-$ where $\hat{V} = V(r')^2$, where $r' \equiv \frac{\partial r}{\partial y}$ and $r_+ = r(y = 1)$ and $r_- = r(y = 0)$.

2. $U, V, r > 0$ throughout the region $r_- < r < r_+$.

3. The loci $r = r_-$ and $r = r_+$ are regular.

4. $G^0_0 = 8\pi T^0_0$ where $T^0_0 = -\rho$ and $\rho(r)$ is the energy density of the material in the manifold.

[2] I am indebted to Jim York, Werner Israel, Jorma Louko, and Don Page for discussions on this point. A full discussion on how to treat the surface term at the horizon is given in Chapter 4.

The first condition assures that there is a cosmological horizon at $r = r_+$ and possibly a black hole horizon at $r = r_-$. The second condition ensures that the region between the two horizons is regular with Euclidean signature. The third condition imposes regularity at the horizon(s). The fourth condition assures that the spacetime satisfies the Einstein energy constraint.

One of the obstacles to arriving at a consistent thermodynamic treatment of spacetimes with two horizons has been the fact that one must ascribe to each horizon its own independent temperature. How a state of thermal equilibrium is possible in such a spacetime has not been clear.

In the Euclidean sector, the temperature of a horizon is fixed by imposing regularity at the horizon (i.e. choosing a limiting form of the lapse function that ensures no conical singularity occurs at the horizon). The problem presented by a two horizon manifold is that one must satisfy two independent regularity conditions.

The condition for regularity at r_+ and r_- is

$$\left[V^{\frac{1}{2}}\left(U^{\frac{1}{2}}\right)'\right]\Big|_{r_\epsilon} = -\epsilon, \tag{2.2}$$

where $\epsilon = \pm 1$. These conditions constrain the lapse function, $\sqrt{U(y)}$, to have the limiting forms,

$$\begin{aligned} \sqrt{U}_{y\to 0} &= \lim_{y\to 0} 2\left[\frac{\partial \hat{V}}{\partial r}\right]^{-1}\sqrt{\hat{V}} \\ \sqrt{U}_{y\to 1} &= \lim_{y\to 1} -2\left[\frac{\partial \hat{V}}{\partial r}\right]^{-1}\sqrt{\hat{V}}. \end{aligned} \tag{2.3}$$

The local inverse temperature is just the local period of the Euclidean time variable,

$$\beta(r) = 2\pi U(r)^{\frac{1}{2}}. \tag{2.4}$$

For the vacuum Schwarzschild–de Sitter solution, one can show that it is not possible in general to impose regularity at both horizons. The vacuum Schwarzschild–de Sitter solution has $\hat{V} = V = (1 - \frac{2M}{r} - \frac{\Lambda r^2}{3})$ and U = const. × V. Since, in general, $\left.\frac{\partial \hat{V}}{\partial r}\right|_{r_-} \neq -\left.\frac{\partial \hat{V}}{\partial r}\right|_{r_+}$, regularity cannot be imposed simultaneously at both horizons.

On the other hand, if one introduces a matter distribution into the spacetime, and solves Einstein's equations, one obtains,

$$\begin{aligned} \hat{V} &= 1 - \frac{2m(r)}{r} - \frac{\Lambda r^2}{3} \\ U &= e^{2\psi}\hat{V}, \end{aligned} \tag{2.5}$$

where

$$m(r) = \int_{r_-}^{r} 4\pi r^2 \rho(r) dr,$$

$$\frac{\partial \psi}{\partial r} = \frac{4\pi r(\rho + p)}{1 - \frac{2m}{r} - \frac{\Lambda r^2}{3}}.$$

Thus, when matter is present, its energy and pressure distribution can be arranged so that U has the correct limiting forms at both $y = 0$ and $y = 1$. Such a distribution is a state of gravitational thermal equilibrium: the local temperature due to the black hole horizon equals the local temperature due to the cosmological horizon.

While I have argued that thermal equilibrium may persist in a classical two horizon spacetime so long as a matter distribution is present, the results which follow are not confined to classical spacetimes (ie. spacetimes for which $G^a_b = 8\pi T^a_b$). The results hold equally for any spacetime which has a metric of the form (2.1) and satisfies the four general conditions set out above. Expression (2.4) defines the local temperature for any such spacetime.

The Euclidean action for a general manifold with boundary is

$$I = -\frac{1}{16\pi}\int_{\mathcal{M}}\Big(R - 2\Lambda\Big)\sqrt{g}d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}}\Big(K - K_0\Big)\sqrt{h}d^3x + I_{\text{matter}}, \tag{2.6}$$

where K is the extrinsic curvature on the boundary, K_0 is the extrinsic curvature on a Minkowski background and I_{matter} is the action of the matter fields. The manifolds of interest here have no boundary (the loci $r = r_+$ and r_- are regular regions of the manifold), so the boundary correction terms in (2.6) are not relevant. Also, without loss of generality, assume that the cosmological constant is zero. [The case of non-zero cosmological constant may be retrieved by ascribing a constant energy density $\rho_{vac} = \frac{\Lambda}{8\pi}$ to the vacuum.] The action may then be written as,

$$I = -\frac{1}{16\pi}\int R\sqrt{g}d^4x + I_{\text{matter}}. \tag{2.7}$$

The scalar curvature associated with metric (2.1) is

$$R = -\frac{1}{\sqrt{g}}\Big(\sqrt{g}V\frac{U'}{U}\Big)' - 2G^0_0. \tag{2.8}$$

The Euclidean action of the matter is given by [4]–[5],

$$I_{\text{matter}} = \int \omega\sqrt{g}d^4x, \tag{2.9}$$

where ω is the local grand potential per unit volume defined by,

$$\omega = \rho - T\sigma - \mu_a n_a, \tag{2.10}$$

where σ is the entropy density and n_a is the number density of any conserved quantity (eg. charge, baryon number, *etc.*).

Now set $G^0_0 = -8\pi\rho$ to obtain,

$$\begin{aligned} I &= \frac{1}{16\pi}\int\Big(\sqrt{g}V\frac{U'}{U}\Big)'d^4x - \int(T\sigma + \mu_a n_a)\sqrt{g}d^4x \\ &= \frac{1}{4}\int\Big[r^2\frac{V^{\frac{1}{2}}}{U^{\frac{1}{2}}}U'\Big]\Big|_{r_-}^{r_+}d\tau - \int(\sigma + \beta\mu_a n_a)\sqrt{^{(3)}g}d^3x, \end{aligned} \tag{2.11}$$

where (2.4) was used in the second equation. Further, by the principle of equivalence, the chemical potential must scale in the same way as the temperature [4],

$$\mu_a = \frac{\alpha_a}{2\pi} U^{-\frac{1}{2}}, \tag{2.12}$$

where $\alpha_a \equiv \frac{\mu_a}{T}$ the 'thermal potential' is constant. Let N_a represent the total number of the conserved quantity a and use the regularity conditions to obtain,

$$I = -\pi r_+^2 - \pi r_-^2 - S_{\text{matter}} - \alpha_a N_a. \tag{2.13}$$

The first two terms on the right hand side of equation (2.13) represent the entropies of the cosmological and black hole horizon respectively so,

$$I = -S_{\text{total}} - \alpha_a N_a, \tag{2.14}$$

where $S_{\text{total}} = S_{\text{bh}} + S_{\text{cosm.}} + S_{\text{matter}}$.

Recall that the grand canonical partition function has a weighting function $e^{-\Phi}$ where the weighting factor Φ is given by

$$\Phi = \beta\omega = \beta E - S - \alpha_a N_a. \tag{2.15}$$

Comparison of equations (2.14) and (2.15) reveals that $I = \Phi$ so long as the mean thermal energy of a compact manifold without boundary is zero.

Some insight into the statistical mechanics of manifolds with cosmological horizons can be obtained by placing a shell with fixed temperature at some r_0 which is between r_- and r_+.

The action for the region inside the shell has been calculated by Martinez and York [4]. To obtain the result, substitute into (2.6)

$$\begin{aligned} \frac{1}{8\pi}\int_{r_0} K\sqrt{h}d^3x &= -\frac{1}{8\pi}V^{\frac{1}{2}}\frac{\partial}{\partial y}\int_{r_0}\sqrt{h}d^3x = -\beta_0 r_0 \hat{V}^{\frac{1}{2}} - \frac{1}{2}r^2 V^{\frac{1}{2}}\left(U^{\frac{1}{2}}\right)'\Big|_{r_0}, \\ \frac{1}{8\pi}\int_{r_0} K_0\sqrt{h}d^3x &= -\frac{1}{8\pi}\int_{r_0}\frac{2}{r}\sqrt{h}d^3x = -\beta_0 r_0. \end{aligned} \tag{2.16}$$

One obtains,

$$I_{\text{int.}} = \beta_0 E_0 - S_{\text{total}} - \alpha_a N_a, \tag{2.17}$$

where

$$E_0 = r_0\Big[1 - \hat{V}^{\frac{1}{2}}(r_0)\Big], \tag{2.18}$$

is the mean thermodynamic energy of the region inside the shell, $S_{\text{total}} = \pi r_-^2 + S_{\text{matter}}$, is the total entropy inside the shell, and N_a is the number of the conserved quantity a inside the shell. Martinez and York interpret (2.17) as the inverse temperature of the shell times the grand potential of the black hole and matter inside.

Now consider the region exterior to the shell (ie. $r_0 < r < r_+$). By a similar calculation to those discussed above, one obtains,

$$I_{\text{ext.}} = -\beta_0 r_0\Big[1 - \hat{V}^{\frac{1}{2}}(r_0)\Big] - \hat{S}_{\text{total}} - \alpha_a \hat{N}_a, \tag{2.19}$$

where $\hat{N}_a$ is the total number of the conserved quantity a outside the shell and $\hat{S}_{\text{total}} = \pi r_+^2 + \hat{S}_{\text{matter}}$ is the sum of the entropy of the cosmological horizon and the matter outside the shell. If one is to relate (2.19) to the grand potential, one must ascribe to the region outside the shell a *negative* mean thermal energy

$$\hat{E}_0 = -r_0\Big[1 - \hat{V}^{\frac{1}{2}}(r_0)\Big]. \tag{2.20}$$

In a sense, this result is not surprising. The mean thermal energy is given by a surface integral over the boundary of the manifold. One might imagine a manifold without boundary as a limiting case of a manifold with boundary in which the 3-volume of the boundary goes to zero. So long as the integrand of the energy surface integral remains finite in this limit, one would ascribe a zero mean thermal energy to a manifold without boundary. Then the energy of the region with $r > r_0$ should simply be the negative of the energy of the region with $r < r_0$[3].

[3] I am indebted to Jim York and Werner Israel for this observation.

One may also calculate the Euclidean action between two concentric spherical shells each at its own fixed temperature. Letting the inner shell be at $r = r_0$ and the outer one at $r = r_1$ yields,

$$I = \beta_0 \hat{E}_0 + \beta_1 E_1 - S_{\text{matter}} - \alpha_a N_a, \tag{2.21}$$

where $\hat{E}_0$ is given by (2.20) and E_1 is given by (2.18) evaluated at r_1.

Fixing the radial positions of the horizons is equivalent to placing bounding shells at r_+ and r_-. The Euclidean action for this case is

$$I = -S_{\text{matter}} - \alpha_a N_a. \tag{2.22}$$

Note that equation (2.22) representing the Euclidean action for a manifold with fixed cosmological and black hole horizons, differs from (2.14) the Euclidean action for the manifold with variable horizons only by the sum of the entropies of the horizons.

In summary, I have shown that a classical spacetime with a cosmological and black hole horizon may be in thermal equilibrium so long as a matter distribution is present. Furthermore, I have calculated the Euclidean action for general (non-classical) spherically symmetric manifolds. It is found to equal the grand-canonical weighting factor so long as the mean thermal energy is taken to be zero. Finally, I have considered how the Euclidean action is modified by the imposition of fixed temperature shells. The mean thermal energy of the cosmological horizon is negative.

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CHAPTER 3

THE FIRST LAW AND HORIZON THERMODYNAMICS

3.1 Introduction

An[1] understanding of the thermodynamic properties of spacetimes with horizons is pivotal to many problems in cosmology. Perhaps one of the most exciting applications of horizon thermodynamics is to problems in quantum cosmology. In recent times, the connections between horizon thermodynamics and quantum cosmology have become increasingly clear [1,2]. The point of contact between these two apparently disparate subjects is the Euclidean action.

In 1977, Gibbons and Hawking [3] pointed out the connection between Euclidean gravitational path integral and the grand canonical partition function. A consequence is that in the 'zero-loop' approximation

$$I = \beta F, \tag{3.1.1}$$

where I is the classical gravitational action, β is inverse temperature and F is the grand canonical free energy. [Units are chosen such that $\hbar = G = c = k = 1$.]

While the Gibbons-Hawking result was intriguing, it was not at all clear how to apply it to real gravitational systems—in particular, bounded systems which include a matter distribution. An important advance was made when York [4] extended the treatment of Gibbons and Hawking to a Schwarzschild black hole enclosed in a spherical shell. Since then, Martinez and York [5] have made further generalizations by calculating the Euclidean action for bounded spacetimes which include both a black hole and a matter distribution. Recently the Euclidean action

[1] A version of this paper will appear in *Physical Review D* (1990).

has been calculated for systems having a matter distribution and either one or both of a cosmological horizon and a black hole horizon [6].

In this paper, I use the connection between the Euclidean action and the free energy to develop a well defined treatment of the thermodynamics of systems including both a horizon and a matter distribution. In particular, I derive the first law of thermodynamics for such systems and evaluate heat capacities when either the area of a bounding shell or its surface pressure are kept fixed. In section 2, I treat systems consisting of a black hole and a matter distribution. Section 3 treats systems which include a matter distribution and a cosmological horizon. Section 3 also discusses the case in which the cosmological constant is allowed to vary.

3.2 Systems with a black hole horizon and a matter distribution

In this section, I consider systems consisting of a black hole and a matter distribution enclosed in a spherical bounding shell. For simplicity, I assume the black hole to be uncharged and not rotating. The problem is to derive the thermodynamic properties of the system. Important insight can be gained by considering the Euclidean action of the system.

A point that was often overlooked in the literature is that the appropriate gravitational action for a system depends critically on whether one constrains metric components, h_{ij}, or their conjugate momenta. The momenta conjugate to h_{ij} are given by

$$\pi^{ij} \equiv \frac{\delta \mathcal{L}_{\text{grav.}}}{\delta \dot{h}_{ij}} = \frac{1}{16\pi} h^{\frac{1}{2}} \left(K^{ij} - h^{ij} K \right) \tag{3.2.1}$$

where $\mathcal{L}_{\text{grav.}}$ is the gravitational Lagrangian and K_{ij} is the extrinsic curvature tensor. If one wishes to constrain π^{ij} on the boundary, the appropriate gravitational action is just

$$I_{\text{grav.}} = -\frac{1}{16\pi}\int_{\mathcal{M}} R\, g^{\frac{1}{2}}\, d^4x, \tag{3.2.2}$$

On the other hand, when one constrains the intrinsic three metric components on the boundary, an additional term must be included in the action so that the variational principle is well defined. Furthermore, it is often useful (though strictly unnecessary) to renormalize the action so that flat spacetime will have zero action [3]. In this case, the gravitational action becomes,

$$I_{\text{grav.}} = -\frac{1}{16\pi}\int_{\mathcal{M}} R g^{\frac{1}{2}}\, d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}} \left[K - K_0\right] h^{\frac{1}{2}}\, d^3x, \tag{3.2.3}$$

where K_0 is the renormalizing constant (equal to the trace of the extrinsic curvature of the boundary in a flat background).

Martinez and York [5] have calculated Euclidean action for systems involving a black hole and a matter distribution when the components of the intrinsic three metric are fixed on the boundary (ie. ones for which (3.2.3) is appropriate). Physically, their choice corresponds to fixing the temperature and surface area of the bounding shell. I now review this calculation as it applies to metrics satisfying Einstein's equations $G_{\mu\nu} = 8\pi T_{\mu\nu}$.

In the Euclidean sector, spherically symmetric systems including both a black hole and a matter distribution may be described by metrics of the form

$$ds^2 = U(r)\, d\tau^2 + V^{-1}(r)\, dr^2 + r^2\, d\Omega^2, \tag{3.2.4}$$

where τ is periodic with period 2π and the radial parameter r extends from a black hole horizon at r_- to a bounding shell at r_1. To obtain a horizon at r_-, we require $U = V = 0$ there. To ensure that the horizon is regular we require,

$$\left[V^{\frac{1}{2}}\left(U^{\frac{1}{2}}\right)'\right]_{r_-} = 1, \tag{3.2.5}$$

where the prime symbol indicates differentiation with respect to r. Imposing Einstein's equations under these constraints, we obtain

$$\begin{aligned} V &= 1 - \frac{r_-}{r} - \frac{8\pi \int_{r_-}^{r} \rho r^2\, dr}{r} \\ U &= \frac{4r_-^2\, e^{2\psi(r)-2\psi(r_-)}}{\left(1 - 8\pi\rho(r_-)\, r_-^2\right)^2} V \\ \frac{\partial\psi}{\partial r} &= \frac{4\pi r(\rho + p)}{V} \end{aligned} \qquad (3.2.6)$$

where $\rho = -\langle T_0^0 \rangle$ and $p = \langle T_1^1 \rangle$.

Local thermodynamics we take to be described by

$$\rho + p = \beta^{-1}\sigma + \mu_j n_j, \qquad (3.2.7)$$

where $\beta(r)$ is the local inverse temperature of the matter, $\sigma(r)$ is its entropy density, $n_j(r)$ are the number densities associated with conserved quantities (eg. charge, baryon number, etc), and $\mu_j(r)$ are the local chemical potentials. The action associated with the matter is then [5],

$$I_{\text{matter}} = \int_{\mathcal{M}} \left(\rho - \beta^{-1}\sigma - \mu_j n_j\right) g^{\frac{1}{2}}\, d^4x, \qquad (3.2.8)$$

Noting that the scalar curvature associated with metric (3.2.4) is,

$$R = -\frac{1}{g^{\frac{1}{2}}} \left(g^{\frac{1}{2}} V \frac{U'}{U} \right)' - 2G_0^0. \qquad (3.2.9)$$

and that the boundary correction term is,

$$-\frac{1}{8\pi} \int_{\partial\mathcal{M}} \left[K - K_0\right] h^{\frac{1}{2}}\, d^3x = \left[2\pi U^{\frac{1}{2}} \left(1 - V^{\frac{1}{2}}\right) - \pi r^2 V^{\frac{1}{2}} \left(U^{\frac{1}{2}}\right)' \right]_{r=r_1}, \qquad (3.2.10)$$

one obtains after imposing the regularity condition at r_-,

$$I = 2\pi U_1^{\frac{1}{2}} r_1 \left(1 - V_1^{\frac{1}{2}}\right) - \pi r_-^2 + \int \left(\frac{1}{8\pi} G_0^0 + \rho - \beta^{-1}\sigma - \mu_j n_j\right) g^{\frac{1}{2}}\, d^4x. \qquad (3.2.11)$$

The above expression can be simplified by making use of the Einstein energy constraint, $G_0^0 = -8\pi\rho$. Furthermore, the local inverse temperature, β, is equal to the local period of the Euclidean time variable, $\beta(r) = 2\pi U(r)^{\frac{1}{2}}$. Also, by virtue of the principle of equivalence, the chemical potentials must scale like the temperature, so $\mu_j = \alpha_j \beta^{-1}$, where the α_j are constant.

Equation (3.2.11) now becomes

$$I = \beta_1 r_1 \left(1 - V_1^{\frac{1}{2}}\right) - \pi r_-^2 - \int_{^{(3)}\mathcal{M}} \sigma \sqrt{^{(3)}g}\, d^3x - \alpha_j \int_{^{(3)}\mathcal{M}} n_j \sqrt{^{(3)}g}\, d^3x, \qquad (3.2.12)$$

where the final integrals are over the spatial three volume of the manifold. Now recall that

$$I = \beta F = \beta E - S - \alpha_j N_j. \qquad (3.2.13)$$

Comparing (3.2.12) with (3.2.13), suggests that the basic thermodynamic variables of the system are

$$E = r_1 \left(1 - V_1^{\frac{1}{2}}\right) \qquad (3.2.14)$$

$$S = S_{\text{bh}} + S_{\text{matter}} = \pi r_-^2 + \int_{^{(3)}\mathcal{M}} \sigma \sqrt{^{(3)}g}\, d^3x \qquad (3.2.15)$$

$$A = 4\pi r_1^2 \qquad (3.2.16)$$

$$N_j = \int_{^{(3)}\mathcal{M}} n_j \sqrt{^{(3)}g}\, d^3x. \qquad (3.2.17)$$

a) The First Law

Having derived equation (3.2.12), Martinez and York concentrate on the special case when the matter in the system is confined to an infinitely thin shell. They attempt to distinguish between the thermodynamic properties of the black hole and those of the matter shell. They find that if the matter shell is placed at the boundary of the system, the energies and surface pressures of black hole and matter decouple. Otherwise, they find that neither the energies nor surface pressures may be separated in any simple way.

Here, I initiate a different approach to treating the thermodynamics of black hole/matter systems. I allow for generic spherically symmetric matter distributions and, in general, do not attempt to distinguish between the thermodynamic properties of the black hole and the matter. My initial objective is to derive the first law.

Note that $E, S, A,$, and N_j in (3.2.17) are independent functions of the thermal potentials α_j and the boundary data r_1, and β_1. Hence, E may be expressed as a function of S, A and N_j and an infinitesimal change in the mean internal energy can be expressed in terms of the identity;

$$dE = \left(\frac{\partial E}{\partial S}\right)_{N_j,A} dS + \left(\frac{\partial E}{\partial A}\right)_{S,N_j} dA + \sum_i \left(\frac{\partial E}{\partial N_i}\right)_{S,A,N_{j\neq i}} dN_i, \tag{3.2.18}$$

where it is understood that all of the N_j are to be held fixed when evaluating the first two terms and all of the N_j except N_i are fixed in the final terms. To ascribe thermodynamic significance to the above identity, it remains to evaluate the partial derivatives on the right hand side.

Before tackling this problem, it is worth noting that by virtue of the regularity condition at the horizon and the limiting behavior of U and V as one approaches the horizon,

$$\begin{aligned} \left.\frac{\partial U}{\partial r}\right|_{r=r_-} &= 2\left[\frac{U_-}{V_-}\right]^{\frac{1}{2}} \\ \left.\frac{\partial V}{\partial r}\right|_{r=r_-} &= 2\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}, \end{aligned} \tag{3.2.19}$$

where a minus sign subscript indicates that the function is to be evaluated on the horizon. Also note that,

$$\left(\frac{\partial V}{\partial r_-}\right)_r = -\frac{2r_-}{r}\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}. \tag{3.2.20}$$

Finally note that,

$$\begin{aligned}
\beta(\rho + p) &= \sigma + \alpha_j n_j \\
&= \frac{U^{\frac{1}{2}}}{4}\left[G^1_1 - G^0_0\right] \\
&= \frac{V^{\frac{3}{2}}}{2r}\frac{\partial}{\partial r}\left[\frac{U}{V}\right]^{\frac{1}{2}}.
\end{aligned} \tag{3.2.21}$$

With the benefit of the above, now consider the quantity $\left(\frac{\partial E}{\partial S}\right)_{N_j,A}$. This may be expressed as

$$\left(\frac{\partial E}{\partial S}\right)_{N_j,A} = \left(\frac{\partial E}{\partial r_-}\right)_{N_j,A}\left(\frac{\partial S}{\partial r_-}\right)^{-1}_{N_j,A}. \tag{3.2.22}$$

Furthermore, one has

$$\begin{aligned}
\left(\frac{\partial E}{\partial r_-}\right)_{N_j,A} &= -\frac{r_1}{2V_1^{\frac{1}{2}}}\left(\frac{\partial V_1}{\partial r_-}\right)_{N_j,A} \\
&= \frac{r_-}{V_1^{\frac{1}{2}}}\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}},
\end{aligned} \tag{3.2.23}$$

where the final equality makes use of (3.2.20). Meanwhile,

$$\begin{aligned}
\left(\frac{\partial S}{\partial r_-}\right)_{A,N_j} &= 2\pi r_- + 4\pi\frac{\partial}{\partial r_-}\left[\int_{r_-}^{r_1}\frac{\sigma r^2}{V^{\frac{1}{2}}}\,dr\right]_{N_j,A} \\
&= 2\pi r_-\left[1 + \left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\frac{2r\sigma}{V^{\frac{3}{2}}}\,dr - \frac{2\sigma(r_-)r_-}{V_-^{\frac{1}{2}}}\right]_{N_j,A}.
\end{aligned} \tag{3.2.24}$$

The last two terms in (3.2.24) should be interpreted as being evaluated in the limit $r \to r_-$. In this limit, they are each divergent if $\sigma(r_-) \neq 0$, but we shall see that these divergences cancel.

Expression (3.2.24) can be simplified by noting that

$$\begin{aligned}
\left(\frac{\partial N_j}{\partial r_-}\right)_{A,N_j} = 0 &= 4\pi\frac{\partial}{\partial r_-}\int_{r_-}^{r_1}\frac{n_j r^2}{V_-^{\frac{1}{2}}}\,dr \\
&= -4\pi\frac{n_j(r_-)r_-^2}{V_-^{\frac{1}{2}}} + 4\pi r_-\left[\frac{V(r_-)}{U(r_-)}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\frac{n_j r}{V^{\frac{3}{2}}}\,dr.
\end{aligned} \tag{3.2.25}$$

Also, from (3.2.21),

$$2\int_{r_-}^{r_1} \frac{r(\sigma+\alpha_j n_j)}{V^{\frac{3}{2}}}\,dr = \left[\frac{U_1}{V_1}\right]^{\frac{1}{2}} - \left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}. \tag{3.2.26}$$

Hence, using (3.2.25) and (3.2.26),

$$2\int_{r_-}^{r_1} \frac{r\sigma}{V^{\frac{3}{2}}}\,dr = \left[\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}} - \left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}\left[1+\frac{2\alpha_j n_j(r_-)r_-}{V_-^{\frac{1}{2}}}\right]\right]. \tag{3.2.27}$$

Substituting (3.2.27) into expression (3.2.24) yields,

$$\left(\frac{\partial S}{\partial r_-}\right)_{A,N_j} = 2\pi r_-\left[\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}} - \frac{2\big(\sigma(r_-)+\alpha_j n_j(r_-)\big)r_-}{V_-^{\frac{1}{2}}}\right]. \tag{3.2.28}$$

But,

$$\begin{aligned} \frac{2r_-\big(\sigma(r_-)+\alpha_j n_j(r_-)\big)}{V_-^{\frac{1}{2}}} &= V_-\frac{\partial}{\partial r}\left[\frac{U}{V}\right]^{\frac{1}{2}}\Bigg|_{r=r_-} \\ &= \frac{1}{2}\left[\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}U'_- - \left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}V'_-\right] \\ &= 0, \end{aligned} \tag{3.2.29}$$

by virtue of (3.2.19). So the expression for $\left(\frac{\partial S}{\partial r_-}\right)_{A,N_j}$ simplifies to

$$\left(\frac{\partial S}{\partial r_-}\right)_{A,N_j} = 2\pi r_-\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}}. \tag{3.2.30}$$

Combining expressions (3.2.23) and (3.2.30) yields the remarkably simple result,

$$\left(\frac{\partial E}{\partial S}\right)_{A,N_j} = \frac{1-8\pi\rho(r_-)r_-^2}{4\pi r_-\sqrt{1-\frac{2m(r_1)}{r_1}}}e^{\psi(r_-)-\psi(r_1)} = \left[2\pi U_1^{\frac{1}{2}}\right]^{-1}. \tag{3.2.31}$$

Recalling that the inverse temperature is given by $\beta \equiv 2\pi U^{\frac{1}{2}}$, one has

$$\left(\frac{\partial E}{\partial S}\right)_{A,N_j} = \beta(r_1)^{-1} = T(r_1), \tag{3.2.32}$$

where $T(r_1)$ is the temperature measured at the surface of the box.

Now consider the terms $\left(\frac{\partial E}{\partial N_i}\right)_{A,N_{j\neq i},S}$ in (3.2.18). Note that,

$$\left(\frac{\partial E}{\partial N_i}\right)_{A,N_{j\neq i},S} = \left(\frac{\partial E}{\partial r_-}\right)_{A,N_{j\neq i},S}\left(\frac{\partial N_i}{\partial r_-}\right)^{-1}_{A,N_{j\neq i},S}. \tag{3.2.33}$$

Further note

$$\begin{aligned}\left(\frac{\partial N_i}{\partial r_-}\right)_{A,N_{j\neq i},S} &= 4\pi\frac{\partial}{\partial r_-}\int_{r_-}^{r_1}\frac{n_i r^2}{V^{\frac{1}{2}}}\,dr \\ &= 2\pi r_-\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\frac{2n_i r}{V^{\frac{3}{2}}}\,dr - 4\pi r_-^2\frac{n_i(r_-)}{V_-^{\frac{1}{2}}}.\end{aligned} \tag{3.2.34}$$

To evaluate the integral in (3.2.34) when S and all N_j except N_i are fixed, consider that

$$\left(\frac{\partial S}{\partial r_-}\right)_{S,A,N_{j\neq i}} = 0 = 2\pi r_-\left[1+\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\frac{2\sigma r}{V^{\frac{3}{2}}}\,dr - \frac{2\sigma(r_-)r_-}{V_-^{\frac{1}{2}}}\right], \tag{3.2.35}$$

so that

$$\left[\frac{U_-}{V_-}\right]^{\frac{1}{2}} = -\int_{r_-}^{r_1}\frac{2\sigma r}{V^{\frac{3}{2}}}\,dr + \left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}\frac{2\sigma(r_-)r_-}{V_-^{\frac{1}{2}}}. \tag{3.2.36}$$

Similarly,

$$\left(\frac{\partial N_j}{\partial r_-}\right)_{S,A,N_{j\neq i}} = 0 = 4\pi r_-\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\frac{n_j r}{V^{\frac{3}{2}}}\,dr - 4\pi r_-^2\frac{n_j(r_-)}{V_-^{\frac{1}{2}}}. \tag{3.2.37}$$

Also, appealing to equation (3.2.21), one has

$$\int_{r_-}^{r_1}\frac{2r(\sigma+\alpha_j n_j)}{V^{\frac{3}{2}}}\,dr = \left[\frac{U}{V}\right]^{\frac{1}{2}}\Bigg|_{r_-}^{r_1}, \tag{3.2.38}$$

where a sum over all j is implied. So, by virtue of equations (3.2.34), (3.2.36), (3.2.37) and (3.2.38), one obtains

$$\begin{aligned}\left(\frac{\partial N_i}{\partial r_-}\right)_{A,N_{j\neq i},S} &= \frac{2\pi r_-}{\alpha_i}\left[\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}} - \frac{2\left(\sigma(r_-)+\alpha_k n_k(r_-)\right)r_-}{V_-^{\frac{1}{2}}}\right] \\ &= \frac{2\pi r_-}{\alpha_i}\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}},\end{aligned} \tag{3.2.39}$$

which combines with (3.2.23) to yield the simple result,

$$\left(\frac{\partial E}{\partial N_i}\right)_{A,N_{j\neq i},S} = \alpha_i\left[2\pi U_1^{\frac{1}{2}}\right]^{-1} = \alpha_i T(r_1) = \mu_i(r_1). \tag{3.2.40}$$

Thus, $\left(\frac{\partial E}{\partial N_i}\right)_{A,N_{j\neq i},S}$ is just the i'th chemical potential of the system as measured at r_1.

The remaining term on the right hand side of (3.2.18) may be calculated in a similar fashion. Specifically,

$$\left(\frac{\partial E}{\partial A}\right)_{N_j,S} = \frac{1}{8\pi r_1}\left[1 - V_1^{\frac{1}{2}} - \frac{r_1}{2V_1^{\frac{1}{2}}}\frac{\partial}{\partial r_1}\left(1 - \frac{r_- + 8\pi\int_{r_-}^{r_1}\rho r^2\,dr}{r_1}\right)_{N_j,S}\right]$$
$$= \frac{1}{8\pi r_1}\left[1 - V_1^{\frac{1}{2}} - \frac{r_1}{2V_1^{\frac{1}{2}}}\left.\frac{\partial V}{\partial r}\right|_{r_1} - \frac{r_1}{2V_1^{\frac{1}{2}}}\left(\frac{\partial V_1}{\partial r_-}\right)\left(\frac{\partial r_-}{\partial r_1}\right)_{N_j,S}\right]. \tag{3.2.41}$$

Taking the derivatives of S and N_j with respect to r_1 and setting them equal to zero, one obtains,

$$\left(\frac{\partial r_-}{\partial r_1}\right)_{N_j,S} = -\frac{r_1 V_1}{r_-}\left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}\left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\left[\frac{\partial}{\partial r}\left[\frac{U}{V}\right]^{\frac{1}{2}}\right|_{r_1}\Bigg]. \tag{3.2.42}$$

Substituting (3.2.42) into (3.2.41) and making use of (3.2.20), one obtains,

$$\left(\frac{\partial E}{\partial A}\right)_{N_j,S} = \frac{1}{8\pi r_1}\left[1 - V_1^{\frac{1}{2}} - \frac{r_1}{2V_1^{\frac{1}{2}}}\left.\frac{\partial V}{\partial r}\right|_{r_1} - r_1 V_1^{\frac{1}{2}}\left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\frac{\partial}{\partial r}\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}}\right|_{r_1}\Bigg] \tag{3.2.43}$$
$$= \frac{1}{8\pi r_1}\left[1 - V_1^{\frac{1}{2}}\left[1 + \frac{r_1}{2U_1}\left.\frac{\partial U}{\partial r}\right|_{r_1}\right]\right] \equiv -\lambda, \tag{3.2.44}$$

where λ is the "surface pressure" found by York [4] generalized to account for the presence of a matter distribution.

Thus, after some work, we arrive at the first law of thermodynamics for spherically symmetric spacetimes including a black hole and a matter distribution bounded by a spherical shell,

$$dE = T\,dS + \mu_j\,dN_j - \lambda\,dA, \tag{3.2.45}$$

where it is understood that all thermodynamic quantities are to be evaluated at the bounding shell and are given by equations (3.2.14) through (3.2.17), as well as by (3.2.32), (3.2.40), and (3.2.44). This law is an essential element in calculations of further thermodynamic quantities.

The above treatment is readily generalized to account for a non-zero cosmological constant, Λ. Einstein's equations in the presence of a cosmological constant become $G_{\mu\nu} = 8\pi T_{\mu\nu} - \Lambda g_{\mu\nu}$. The spherically symmetric metric satisfying these equations is just (3.2.4) with

$$\begin{aligned} V &= 1 - \frac{r_-}{r} - \frac{8\pi \int_{r_-}^{r} (\rho + \rho_\Lambda) r^2 \, dr}{r} \\ U &= \frac{4r_-^2 e^{2(\psi(r) - \psi(r_-))}}{\left(1 - 8\pi(\rho_- + \rho_\Lambda) r_-^2\right)^2} V \end{aligned} \tag{3.2.46}$$

and

$$\frac{\partial \psi}{\partial r} = \frac{4\pi(\rho + p) r}{V}, \tag{3.2.47}$$

where $\langle T_0^0 \rangle = -\rho$ and $\langle T_1^1 \rangle = p$ and $\rho_\Lambda = \frac{\Lambda}{8\pi}$. These metric components can be obtained from equations (3.2.6) by substituting everywhere $\rho + \rho_\Lambda$ for ρ and substituting $p - \rho_\Lambda$ for p.

We wish to fix the temperature and surface area of the boundary as well as the cosmological constant. The appropriate gravitational action is

$$I_{\text{grav.}} = -\frac{1}{16\pi} \int_{\mathcal{M}} \left(R - 2\Lambda\right) g^{\frac{1}{2}} \, d^4x - \frac{1}{8\pi} \int_{\partial \mathcal{M}} \left(K - K_0\right) h^{\frac{1}{2}} \, d^3x \tag{3.2.48}$$

The matter action remains unchanged. Calculations similar to those performed above yield

$$I = \beta E - S - \alpha_j N_j, \tag{3.2.49}$$

where E, S, and N_j are as defined in (3.2.14), (3.2.15) and(3.2.17) except that they are now functions of metric components (3.2.46).

Note that inclusion of the cosmological constant does not change the functional form of the action. Inclusion of a cosmological constant does, however, add another term to the first law. Now the mean thermal energy E is a function not only of of S, A, and N_j, but also of ρ_Λ. The infinitesimal variation of E can then be expressed as

$$dE = \left(\frac{\partial E}{\partial S}\right)_{A,N_j,\rho_\Lambda} dS + \left(\frac{\partial E}{\partial A}\right)_{S,N_j,\rho_\Lambda} dA + \left(\frac{\partial E}{\partial N_i}\right)_{A,N_{j\neq i},\rho_\Lambda} dN_j + \left(\frac{\partial E}{\partial \rho_\Lambda}\right)_{S,A,N_j} d\rho_\Lambda. \tag{3.2.50}$$

Consider, the last term in (3.2.50),

$$\left(\frac{\partial E}{\partial \rho_\Lambda}\right)_{S,A,N_j} = -\frac{r_1}{2V_1^{\frac{1}{2}}}\left(\frac{\partial V_1}{\partial \rho_\Lambda}\right)_{A,S,N_j}, \tag{3.2.51}$$

where

$$\left(\frac{\partial V_1}{\partial \rho_\Lambda}\right)_{A,S,N_j} = -\frac{2r_-}{r_1}\left[\frac{V_-}{U_-}\right]^{\frac{1}{2}}\left(\frac{\partial r_-}{\partial \rho_\Lambda}\right)_{A,S,N_j} - \frac{8\pi}{3}\frac{(r_1^3 - r_-^3)}{r_1}. \tag{3.2.52}$$

Using the relations for S and N_j, one obtains,

$$\left(\frac{\partial r_-}{\partial \rho_\Lambda}\right)_{A,S,N_j} = -\frac{4\pi}{3r_-}\left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}\left(r_1^3 - r_-^3\right) + \frac{4\pi}{r_-}\left[\frac{U_-}{V_-}\right]^{\frac{1}{2}}\left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\int_{r_-}^{r_1}\left(\frac{U}{V}\right)^{\frac{1}{2}} r^2\, dr. \tag{3.2.53}$$

Substitute (3.2.52) and (3.2.53) into (3.2.51) to obtain

$$\left(\frac{\partial E}{\partial \rho_\Lambda}\right)_{A,S,N_j} = \frac{4\pi}{U_1^{\frac{1}{2}}}\int_{r_-}^{r_1}\left(\frac{U}{V}\right)^{\frac{1}{2}} r^2\, dr = T(r_1)V^{(4)}, \tag{3.2.54}$$

where $V^{(4)}$ is the four volume of the manifold.

Calculations akin to those performed above yield the other thermodynamic terms in (3.2.50). The first law for black hole/matter systems with a cosmological constant becomes,

$$dE = T\,dS + \mu_j\,dN_j - \lambda\,dA + TV^{(4)}\,d\rho_\Lambda, \tag{3.2.55}$$

where T, μ_j, and λ are as in equations (3.2.32), (3.2.40), and (3.2.44) with U and V now given by (3.2.46).

b) Heat capacity at constant area

Under variations of the system such that the cosmological constant, the particle numbers, and the area of the boundary are held fixed, the relevant heat capacity is,

$$C_{A,N_j,\Lambda} = T\left(\frac{\partial S}{\partial T}\right)_{A,N_j,\Lambda} = \left(\frac{\partial E}{\partial T}\right)_{A,N_j,\Lambda}. \qquad (3.2.56)$$

When evaluating $C_{A,N_j,\Lambda}$, we can without loss of generality set the cosmological constant equal to zero. [The case with non-zero cosmological constant may be retrieved by substituting $\rho + \rho_\Lambda$ for ρ and $p - \rho_\Lambda$ for p in the final expression for C_A.] Furthermore, for simplicity, I will concentrate on the case in which all chemical potentials μ_j are zero so the conserved particle numbers are irrelevant.

Given these conditions, the heat capacity becomes

$$\begin{aligned} C_A &= \left(\frac{\partial E}{\partial r_-}\right)_A \left(\frac{\partial T}{\partial r_-}\right)_A^{-1}, \\ &= \frac{\kappa r_-}{V_1^{\frac{1}{2}}}\left(\frac{\partial T}{\partial r_-}\right)_A^{-1}, \end{aligned} \qquad (3.2.57)$$

where the surface gravity κ is given by $\kappa = \left[\frac{V_-}{U_-}\right]^{\frac{1}{2}} = \frac{1-8\pi\rho r^2}{r}\Big|_{r=r_-}$. Further,

$$\begin{aligned} \left(\frac{\partial T}{\partial r_-}\right)_A &= \frac{\partial}{\partial r_-}\left(\frac{1}{2\pi U_1^{\frac{1}{2}}}\right)_A \\ &= T\left(\frac{\kappa r_-}{r_1 V_1} - \left[\frac{V_1}{U_1}\right]^{\frac{1}{2}} \frac{\partial}{\partial r_-}\left[\int_{r_-}^{r_1} \frac{2r\sigma}{V^{\frac{3}{2}}}\, dr + \frac{1}{\kappa}\right]_A\right) \\ &= T\left[\frac{\kappa r_-}{r_1 V_1} - \left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\left[6\kappa r_- \int_{r_-}^{r_1} \frac{2\sigma}{V^{\frac{5}{2}}}\, dr \right.\right. \\ &\qquad \left.\left. + \frac{\kappa + 4\pi\rho'_- r_-^2 + 8\pi\rho_- r_-}{\kappa^2 r_-}\right]\right], \end{aligned} \qquad (3.2.58)$$

where $\rho'_- \equiv \frac{\partial\rho}{\partial r}\Big|_{r=r_-}$. Hence,

$$C_A = 2\pi\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}}\left[\frac{1}{r_1 V_1} - \left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\left(6\int_{r_-}^{r_1} \frac{\sigma}{V^{\frac{5}{2}}}\, dr + \frac{\kappa + 4\pi\rho'_- r_-^2 + 8\pi\rho_- r_-}{\kappa^3 r_-^2}\right)\right]^{-1}. \qquad (3.2.59)$$

Note that in the vacuum case (3.2.59) reduces to York's expression for the heat capacity [4]:

$$C_A = -2\pi r_-^2 V_1 \left[1 - \frac{3r_-}{2r_1}\right]^{-1}. \tag{3.2.60}$$

For this case, York points out that if r_1 is less than $3M$ the heat capacity is positive and black hole configuration is stable; otherwise, the black hole has negative heat capacity and is thermodynamically unstable.

When matter is present, the condition for the system to have positive heat capacity is

$$r_1 V_1 \leq \frac{\int_{r_-}^{r_1} \frac{2r\sigma}{V^{\frac{3}{2}}}\,dr + \kappa^{-1}}{6\int_{r_-}^{r_1} \frac{\sigma}{V^{\frac{5}{2}}}\,dr + \frac{\kappa + 4\pi\rho'_- r_-^2 + 8\pi\rho_- r_-}{\kappa^3 r_-^2}}. \tag{3.2.61}$$

Note that $\sigma \geq 0$ and $\rho \geq 0$ for matter satisfying the weak energy condition. Similarly, $\kappa > 0$ by virtue of the third law of horizon thermodynamics (ie. the temperature must be positive). If we assume that ρ'_- is also positive, or, at least that,

$$\kappa + 4\pi\rho'_- r_-^2 + 8\pi\rho_- r_- > 0, \tag{3.2.62}$$

then the right hand side of (3.2.61) is positive definite. Furthermore, as $r_1 \to r_-$, the right hand side of (3.2.61) approaches the positive quantity

$$\frac{\kappa^2 r_-^2}{\kappa + 4\pi\rho'_- r_-^2 + 8\pi\rho_- r_-}. \tag{3.2.63}$$

Meanwhile, the left hand side goes to zero as one approaches the horizon. Hence, for an arbitrary matter configuration satisfying (3.2.62), it is always possible to choose a bounding shell small enough that the heat capacity becomes positive.

On the other hand, if one picks an arbitrary radius r_1 for the bounding shell and an arbitrary horizon radius $r_- < r_1$, it should be possible to choose a matter distribution such that the heat capacity of the system is positive. Essentially, this is because the right hand side of (3.2.61) is positive and bounded from below, whereas the left hand side can be made arbitrarily small by including enough matter that $V_1 \to 0$.

An example of a positive heat capacity black hole system which is enclosed in a very large box is obtained if we choose a non-zero cosmological constant or equivalently, choose ρ constant and $\rho = -p$. With this equation of state, a cosmological horizon forms at $r = r_+ \sim \left(\frac{3}{8\pi\rho}\right)^{\frac{1}{2}}$. To avoid having to consider the thermodynamic implications of such a horizon, enclose the system in a box of radius $r_1 < r_+$ and set $\rho = p = 0$ outside the box so no cosmological horizon forms.

In this example, the condition for obtaining a positive heat capacity system is

$$r_1 V_1 \le \frac{r_-}{2} \frac{(1 - 8\pi\rho r_-^2)^2}{(1 + 8\pi\rho r_-^2)}. \tag{3.2.64}$$

When $\rho << r_-^2$, the condition is satisfied if

$$r_1 < \frac{3}{2} r_- + O(r_-^3 \rho), \tag{3.2.65}$$

or if

$$r_1 > r_+ - \frac{1}{4} r_- + O(r_-^3 \rho). \tag{3.2.66}$$

For this specific example, positive heat capacity systems are obtained if the box is either placed close to the black hole horizon or close to a 'would be' cosmological horizon. In general, it is clear from (3.2.61) that a positive heat capacity black hole/matter system can be achieved so long as the density of the matter distribution is sufficiently high.

As a footnote to this discussion, it is interesting to point out that a *formal* distinction can be made between the heat capacity of the black hole and that of the surrounding matter,

$$
\begin{aligned}
C_A &= T\frac{\partial}{\partial T}\Big(S_{\rm bh} + S_{\rm matter}\Big)_A \\
&= T\Big(\frac{\partial S_{\rm bh}}{\partial T}\Big)_A + T\Big(\frac{\partial S_{\rm matter}}{\partial T}\Big)_A = C_{\rm A\ bh} + C_{\rm A\ matter}. \qquad (3.2.67)
\end{aligned}
$$

Furthermore, the ratio of the two heat capacities is given by,

$$
\frac{C_{\rm A\ bh}}{C_{\rm A\ matter}} = \Big(\exp\big[\psi(r_1) - \psi(r_-)\big] - 1\Big)^{-1}. \qquad (3.2.68)
$$

If one includes a matter distribution satisfying the weak energy condition and takes the limit $r_1 \to \infty$ this ratio approaches zero. This is to be expected since for such systems, the matter distribution dominates and

$$
C_A \approx C_{A\ \rm matter}. \qquad (3.2.69)
$$

c) Heat capacity at fixed surface pressure

Since real black holes are not surrounded by rigid spherical shells, one might call into question the cosmological significance of a quantity like C_A.

The alternative to trying to keep the area of the bounding shell fixed would be to fix the surface pressure and allow the area to vary freely. This choice of boundary conditions may more closely approximate the actual boundary conditions on black holes in a quasi-static universe. For instance, one could imagine a membrane surrounding the black hole kept at constant surface pressure by the external universe. [Such a possibility was first suggested by York [4].]

For this case, (3.2.3) is not the appropriate expression for the gravitational action. One is constraining the metric component $h_{\tau\tau}$ and the momenta conjugate to $h_{\theta\theta}$ and $h_{\phi\phi}$. Hence it is necessary to add to (3.2.2) only the term

$$
\int_{\partial\mathcal{M}} \pi^{\tau\tau} h_{\tau\tau}\, d^3x = \frac{1}{16\pi}\int_{\partial\mathcal{M}} \Big(K^{\tau}_{\tau} - K\Big) h^{\frac{1}{2}}\, d^3x. \qquad (3.2.70)
$$

Including the appropriate renormalizing constant, the gravitational action becomes,

$$I_{\text{grav.}} = -\frac{1}{16\pi}\int_{\mathcal{M}} Rg^{\frac{1}{2}}\, d^4x - \frac{1}{16\pi}\int_{\partial\mathcal{M}}\Big[K_i^i - (K_0)_i^i\Big] h^{\frac{1}{2}}\, d^3x, \tag{3.2.71}$$

where $K_i^i = K_\theta^\theta + K_\phi^\phi$.

A calculation akin to the one performed above yields

$$I = \beta F_\lambda = \beta E - S - \alpha_j N_j + \lambda A, \tag{3.2.72}$$

where E, S, A, and N_j are as in (3.2.17) and λ is the surface pressure given in equation (3.2.44). The thermodynamic reason for the appearance of the additional term λA in the free energy is that a transformation has been made to a different ensemble in which fluctuations are allowed in the surface area: the free energy must be modified accordingly. [Such a free energy was proposed by York in Ref. [4].]

The relevant heat capacity for a black hole/matter system held at constant surface pressure is

$$\begin{aligned} C_\lambda &= T\Big(\frac{\partial S}{\partial T}\Big)_\lambda \\ &= T\Big(\frac{\partial S}{\partial r_-}\Big)_\lambda \Big(\frac{\partial T}{\partial r_-}\Big)_\lambda^{-1}. \end{aligned} \tag{3.2.73}$$

Unfortunately, when a matter distribution is present, the expression for C_λ is lengthy and difficult to analyze. Here I derive C_λ for the vacuum case. Much information about the general behavior of C_λ may be gained by considering this relatively simple example.

Note that,

$$\Big(\frac{\partial S}{\partial r_-}\Big)_\lambda = 2\pi r_-, \tag{3.2.74}$$

and

$$\begin{aligned}\left(\frac{\partial T}{\partial r_-}\right)_\lambda &= -4\pi T^2 \frac{\partial}{\partial r_-}\left(r_- V_1^{\frac{1}{2}}\right)_\lambda \\ &= -4\pi T^2\left[V_1^{\frac{1}{2}} + \frac{1}{2} r_- V_1^{-\frac{1}{2}}\left(-\frac{1}{r_1} + \frac{r_-}{r_1^2}\left(\frac{\partial r_1}{\partial r_-}\right)_\lambda\right)\right].\end{aligned} \tag{3.2.75}$$

Holding λ fixed and differentiating expression (3.2.44) with respect to r_-, one finds after some rearranging that

$$\left(\frac{\partial r_1}{\partial r_-}\right)_\lambda = \frac{x}{4}\left[1 - \frac{3}{2}x + \frac{3}{4}x^2 - \left(1-x\right)^{\frac{3}{2}}\right]^{-1}, \tag{3.2.76}$$

where $x \equiv \frac{r_-}{r_1}$. Substituting back into expression (3.2.75) and then into (3.2.73), one obtains,

$$C_\lambda = -2\pi r_-^2(1-x)\left[1 - \frac{3}{2}x + \frac{1}{8}x^3\left(1 - \frac{3}{2}x + \frac{3}{4}x^2 - (1-x)^{\frac{3}{2}}\right)^{-1}\right]^{-1}. \tag{3.2.77}$$

Strictly speaking, C_λ should now be expressed as a function of the fixed quantities λ and β where, for instance,

$$\beta\lambda = \frac{x}{2}\left(\left(1 - \frac{x}{2}\right) - \left(1-x\right)^{\frac{1}{2}}\right). \tag{3.2.78}$$

In order for C_λ to be positive, we require,

$$0 \geq \left[1 - \frac{3}{2}x + \frac{1}{8}x^3\left(1 - \frac{3}{2}x + \frac{3}{4}x^2 - (1-x)^{\frac{3}{2}}\right)^{-1}\right]^{-1}. \tag{3.2.79}$$

Interestingly, there are no values of r_1 such that $r_1 > r_-$ and r_1 satisfies the above condition. In other words, C_λ is negative for all physical choices of λ and β[2].

3.3 Systems with a cosmological horizon and a matter distribution

Now consider systems extending from a fixed area shell at $r = r_1$ out to a cosmological horizon at $r = r_+$.

[2]After completing this work it has come to my attention that this conclusion has been reached in unpublished work by Jim York and collaborators.

The presence of a cosmological horizon implies that $U_+ = V_+ = 0$. Regularity of the horizon requires that

$$\left(\frac{\partial V}{\partial r}\right)\bigg|_{r=r_+} = -2\left[\frac{V_+}{U_+}\right]^{\frac{1}{2}}. \tag{3.3.1}$$

The metric is then given by (3.2.4) with metric components

$$\begin{aligned} V &= 1 - \frac{r_+}{r} + \frac{8\pi \int_r^{r_+} \rho r^2\, dr}{r} \\ U &= \frac{4r_+^2 e^{2((\psi(r)-\psi(r_+))}}{\left(1 - 8\pi(\rho_+ + \rho_\Lambda)r_+^2\right)^2} V \\ \frac{\partial \psi}{\partial r} &= \frac{4\pi(\rho + p)r}{V}. \end{aligned} \tag{3.3.2}$$

The functional expressions for both the gravitational and matter actions are not changed and are given by (3.2.48) and (3.2.8). A calculation of the total action yields [6],

$$I = -\beta r_1\left(1 - V_1^{\frac{1}{2}}\right) - \pi r_+^2 - \int_{^{(3)}\mathcal{M}} \sigma\sqrt{^{(3)}g}\, d^3x - \alpha_j \int_{^{(3)}\mathcal{M}} n_j \sqrt{^{(3)}g}\, d^3x. \tag{3.3.3}$$

Appealing to the fact that $I = \beta F$ in the zero–loop approximation, we obtain the following thermodynamic variables of the system.

$$\begin{aligned} \hat{E} &= -r_1\left(1 - V_1^{\frac{1}{2}}\right) \\ \hat{S} &= S_{ch} + S_{\text{matter}} = \pi r_+^2 + \int_{^{(3)}\mathcal{M}} \sigma\sqrt{^{(3)}g}\, d^3x \\ \widehat{N}_j &= \int_{^{(3)}\mathcal{M}} n_j \sqrt{^{(3)}g}\, d^3x. \end{aligned} \tag{3.3.4}$$

Note that the energy associated with the cosmological horizon $\hat{E}$ is negative [6]; indeed, it is the negative of the expression one obtains for a black hole. Similarly, calculating the surface pressure $\hat{\lambda} = -\left(\frac{\partial \hat{E}}{\partial A}\right)_{\hat{S},\widehat{N}_j,\rho_\Lambda}$, one finds that

$$\hat{\lambda} = \frac{1}{8\pi r_1}\left[1 - V_1^{\frac{1}{2}}\left[1 + \frac{r_1}{2U_1}\frac{\partial U}{\partial r}\bigg|_{r_1}\right]\right] \tag{3.3.5}$$

which is just the negative of expression (3.2.44) for the surface pressure of a black hole system.

The reason why the energy and surface pressure are negative for the cosmological horizon system can be traced to the fact that they are both first order functions of the extrinsic curvature tensor whose sign depends on the direction of the unit normal to the boundary surface. Specifically,

$$\beta E = \frac{1}{16\pi}\int_{\partial\mathcal{M}}\Big(\big(K^{\tau}_{\tau} - K\big) - \big((K_0)^{\tau}_{\tau} - K_0\big)\, h^{\frac{1}{2}}\, d^3x \qquad (3.3.6)$$

and

$$\lambda A = \frac{1}{16\pi}\int_{\partial\mathcal{M}}\Big(\big(K^{i}_{i} - 2K\big) - \big((K_0)^{i}_{i} - 2K_0\big)\, h^{\frac{1}{2}}\, d^3x. \qquad (3.3.7)$$

Since the extrinsic curvature changes sign as one crosses the surface (each side defining the extrinsic curvature using its own outward pointing normal) and since the components of the intrinsic three metric β_1 and r_1 must be continuous, the sign of the energy and surface pressure must change across the surface.

Another way to interpret the negative energy associated with a cosmological horizon is to note that the energy of any closed manifold without boundary is zero [6]. An observer in a manifold extending from a boundary at r_1 to a horizon at r_+ measures the *absence* of the energy of the region $r < r_1$. At the same time, a negative surface pressure is expected because the gravitational force on a stationary object at the boundary is directed radially outward. The shell needs a surface tension to hold itself together [7].

The first law appropriate for systems extending from a boundary to a cosmological horizon can be shown to be

$$d\widehat{E} = T\, d\widehat{S} - \widehat{\lambda}\, dA + \mu_j \widehat{N}_j + T\, V^{(4)}\, d\rho_\Lambda, \qquad (3.3.8)$$

Where T and μ are the same as for the black hole case, $\widehat{E}, \widehat{S}, A$, and $\widehat{N}_j$ are given by (3.3.4) and $\widehat{\lambda}$ is given by (3.3.5).

a) Vacuum de Sitter space

Insight into the significance of equation (3.3.8) may be gained by considering the special example of vacuum de Sitter space. For this case, $\rho = \rho_\Lambda$ and $\frac{8\pi}{3}\rho_\Lambda r_+^2 = 1$. The metric components become

$$\begin{aligned} V &= 1 - \frac{r^2}{r_+^2} \\ U &= r_+^2 V. \end{aligned} \tag{3.3.9}$$

Expression (3.2.32) for the temperature yields

$$T(r) = (2\pi r_+)^{-1}(1 - \frac{r^2}{r_+^2})^{-\frac{1}{2}}, \tag{3.3.10}$$

which is just the standard Hawking temperature normally ascribed to vacuum de Sitter space (corrected for the local Tolman redshift factor).

However, it is not formally correct to refer to (3.3.10) as the local temperature in vacuum de Sitter space. Rather, it should considered as the local temperature measured in a Schwarzschild-de Sitter space in the limit that the mass parameter goes to zero.

There is an important topological distinction between true vacuum de Sitter space and the $M \to 0$ limit of vacuum Schwarzschild-de Sitter space. The essential difference remains even if no Schwarzschild horizon actually occurs. For instance, the manifold could extend from some massive shell out to a cosmological horizon. In the limit that the mass of the shell goes to zero, one does not recover true vacuum de Sitter space.

This is because the presence of a mass parameter, no matter how small, breaks the $O(4)$ symmetry of vacuum de Sitter space. The shell defines a natural $3+1$ symmetry centered on itself. In the absence of such a preferred frame (ie.

in true vacuum de Sitter space) there is no objective significance to the radial position of the horizon.

Thermodynamically the temperature of a system relates to the variation of the entropy with respect to variations of the internal energy. Such variations are well defined only if there exists an independent parameter which can be identified with energy. Equation (3.3.10) relates to the variation of the entropy with respect to energy in the presence of a mass parameter. The mass parameter may then be set equal to zero *after* the variation is taken (in other words, one calculates variations of the mass parameter around a zero value). If there were no mass parameter in the metric it would not be possible to identify an energy for the system and, hence, it would not be strictly correct to speak of the system as having a temperature.

To see this in detail, note that if one were to naively calculate the action associated with a system extending from a bounding shell out to a vacuum de Sitter horizon by setting $M = 0$ at the outset, one would obtain,

$$I = -\beta_1 r_1 \left(1 - \left(1 - \frac{r_1^2}{r_+^2}\right)^{\frac{1}{2}}\right) - \pi r_+^2. \tag{3.3.11}$$

One would be tempted to identify an energy $\hat{E}$ with the quantity

$$-r_1 \left(1 - \left(1 - \frac{r_1^2}{r_+^2}\right)^{\frac{1}{2}}\right). \tag{3.3.12}$$

However, a quick calculation reveals that $\left(\frac{\partial S}{\partial \hat{E}}\right)_A \neq \beta_1$.

The point of this discussion is that while it is correct to identify a temperature associated with the $M \to 0$ limit of Schwarzschild–de Sitter space, it is not strictly correct to ascribe a temperature to vacuum de Sitter space. Nor would it be correct to ascribe a heat capacity to vacuum de Sitter space.

It may seem a little pedantic to stress such a distinction, but considering the confusion that reigns in the treatment of the thermodynamics of de Sitter space, it is an important point of principle. In practice, of course, it would be impossible to ascribe *any* thermodynamic quantity to true de Sitter space since any real observer or real bounding shell would have some mass which would break the $O(4)$ symmetry.

b) Heat capacity at constant area

Even though the energy associated with a cosmological horizon is negative, the condition for thermal stability should still be that the heat capacity be positive. To see this, assume that a system extending from a boundary at r_1 out to a cosmological horizon is hotter than its 'surroundings' (ie. the region with r *less* than the radius of the boundary). The system should radiate resulting in a decrease in its energy density. A decrease in the energy density within the system results in a decrease in V_1 and, hence, causes the energy to become more negative. If the heat capacity at constant surface area is negative, the decrease in energy will be accompanied by an increase in temperature, thus, placing the system even more out of equilibrium with its surroundings[3].

Bearing this in mind, we are now in a position to evaluate the heat capacities associated with a system consisting of a cosmological horizon and a matter distribution. As before, limit attention to the case in which all the α_j are zero.

[3] The above argument implicitly assumes that the temperature of the region interior to r_1 does not change as radiation is emitted into it. This would be the case if $r_+ >> 1$ (in Planck units) and $r_1 \approx r_+$. In fact, it may be possible to have a thermodynamic stable cosmological horizon system even if its heat capacity is negative so long as the temperature of the system increases more slowly than the temperature of the region interior to r_1 as radiation is emitted into this region.

The heat capacity at fixed surface area is then,

$$C_A = -2\pi\left[\frac{U_1}{V_1}\right]^{\frac{1}{2}}\left[\frac{1}{r_1 V_1} + \left[\frac{V_1}{U_1}\right]^{\frac{1}{2}}\left[6\int_{r_1}^{r_+}\frac{\sigma}{V^{\frac{5}{2}}}\,dr + \frac{\kappa - 4\pi\rho_+' r_+^2 - 8\pi\rho_+ r_+}{\kappa^3 r_+^2}\right]\right]^{-1}. \tag{3.3.13}$$

The condition for positive heat capacity is

$$r_1 V_1 \geq \frac{\int_{r_1}^{r_+}\frac{2r\sigma}{V^{\frac{3}{2}}}\,dr - \kappa^{-1}}{6\int_{r_1}^{r_+}\frac{\sigma}{V^{\frac{5}{2}}}\,dr + \frac{\kappa - 4\pi\rho_+' r_+^2 - 8\pi\rho_+ r_+}{\kappa^3 r_+^2}}. \tag{3.3.14}$$

From (3.3.14), it is possible to show that C_A should be negative in the limit $r_1 \to r_+$. In this limit, (3.3.14) becomes

$$r_1 V_1 \geq \frac{r_+(1 - 8\pi\rho_+ r_+^2)^2}{2\left(1 + 8\pi\rho_+ r_+^2\right) + 8\pi\rho_+' r_+^3}. \tag{3.3.15}$$

One expects that ρ_+' is positive. Also, positivity of temperature requires that $8\pi\rho_+ r_+^2 > 1$. Hence, all quantities on the right hand side of (3.3.15) are fixed and positive definite. Meanwhile, the left hand side must approach zero as the the bounding shell approaches the horizon, so it is clear the condition for positive heat capacity must be violated in this limit.

Nonetheless, it should still be possible to construct positive heat capacity solutions with $r_1 \lesssim r_+$ by choosing the surface gravity κ to be arbitrarily close to zero (ie. choosing $8\pi\rho_+ r_+^2 \sim 1$).

For a bounded system which includes a cosmological horizon and can be approximated by the $M \to 0$ limit of a Schwarzschild–de Sitter metric, (3.3.13) becomes

$$C_{A,\rho_\Lambda} = -2\pi r_+\left(\frac{1}{r_1 V_1} - \frac{2}{r_+}\right)^{-1}. \tag{3.3.16}$$

Assuming a breaking of the $O(4)$ symmetry, this is the heat capacity that one would identify with 'vacuum de Sitter space'. The heat capacity is negative regardless of the value of r_1. Furthermore, $C_A \to 0^-$ as $r_1 \to r_+$ or $r_1 \to 0$.

c) Systems at fixed four volume

Until now we have considered systems in which the cosmological constant is held fixed and the four volume was allowed to vary freely. However, there are circumstances under which one might wish to let the cosmological constant vary.

Recently, for instance, Hawking [8] and Coleman [9] have each argued that the Euclidean path integral should be strongly peaked around classical solutions with a cosmological constant equal to zero. While the mechanisms proposed by Hawking and Coleman are quite different, at the core of each of their proposals are certain assumptions about the Euclidean action and how to perform a path integral when the cosmological constant is allowed to vary.

Essentially, they take the classical action for a manifold without boundary

$$I = -\frac{1}{16\pi}\int_{\mathcal{M}}\left(R - 2\Lambda\right) g^{\frac{1}{2}} d^4x, \tag{3.3.17}$$

impose Einstein's equations for vacuum de Sitter space, to obtain

$$I = -\pi r_+^2 = -S_{ch} = -\frac{3\pi}{\Lambda}, \tag{3.3.18}$$

and note that since the path integral has as a weighting factor, e^{-I}, a manifold with zero cosmological constant would be given infinite weight. Despite the fact that such solutions cause radical divergences in the path integral, this is taken to be a mechanism for generating the extremely low observed value for the cosmological constant.

The difficulties with such arguments become clear upon examination of the first law for systems with a cosmological constant (3.2.55). The thermodynamic potential conjugate to ρ_Λ is the four-volume $V^{(4)}$. It is not clear whether Hawking and Coleman intend to consider a statistical ensemble in which the cosmological constant is fixed or an ensemble in which the four-volume is fixed. One might even imagine an ensemble in which neither quantity is fixed. In the absence of such a precise definition of the statistical ensemble, the analysis Hawking and Coleman is ill defined.

For instance, if one considers an ensemble in which the four-volume is constrained, the stationary phase approximations given by Hawkind and Coleman are no longer valid. Essentially, this is due to the fact that when one extremizes an action subject to a constraint, the extremal solution is in general different from that one would obtain if no constraint were present.

I now calculate the classical action (eg. the action relevant to a stationary phase approximation in quantum gravity) for a bounded cosmological horizon/matter system with fixed four-volume and fixed temperature and surface area on the boundary. The total action functional is given by

$$I = -\frac{1}{16\pi}\int_{\mathcal{M}}(R-2\Lambda)g^{\frac{1}{2}}\,d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}}(K-K_0)\,h^{\frac{1}{2}}\,d^3x + I_{\text{matter}}. \qquad (3.3.19)$$

The classical solution will extremize (3.3.19) subject to the condition that

$$\int_{\mathcal{M}} g^{\frac{1}{2}}\,d^4x = V_0^{(4)}, \qquad (3.3.20)$$

where $V_0^{(4)}$ is some fixed four-volume. To extremize (3.3.19) we require that,

$$0 = \Big(G_{\mu\nu} + \Lambda g_{\mu\nu} - 8\pi T_{\mu\nu}\Big)\delta g^{\mu\nu}\,g^{\frac{1}{2}} \qquad (3.3.21)$$

To maintain fixed four-volume, we also require,

$$0 = g_{\mu\nu}\delta g^{\mu\nu}\,g^{\frac{1}{2}}. \qquad (3.3.22)$$

Using the method of Lagrangian undetermined multipliers, the extremization condition becomes,

$$0 = \Big(G_{\mu\nu} + \Lambda g_{\mu\nu} + \widehat{\Lambda} g_{\mu\nu} - 8\pi T_{\mu\nu}\Big), \qquad (3.3.23)$$

where $\hat{\Lambda}$ is an undetermined multiplier to be fixed by condition (3.3.20).

Using equation (3.2.9), and the expression for G_0^0 from equation (3.3.23),

$$\begin{aligned} I &= -\beta_1 r_1 \left((1 - V_1^{\frac{1}{2}} \right) - \pi r_+^2 - \int_{^{(3)}\mathcal{M}} \sigma \sqrt{^{(3)}g}\, d^3x \\ &\qquad - \int_{^{(3)}\mathcal{M}} \alpha_j n_j \sqrt{^{(3)}g}\, d^3x - \frac{\hat{\Lambda}}{8\pi} V_0^{(4)} \\ &= \beta_1 \hat{E} - \hat{S} - \alpha_j \widehat{N}_j - \widehat{\rho_\Lambda} V_0^{(4)}, \end{aligned} \tag{3.3.24}$$

where $\widehat{\rho_\Lambda} = \frac{\hat{\Lambda}}{8\pi}$. The appearance of the additional term $\widehat{\rho_\Lambda} V_0^{(4)}$ is anticipated since the free energy must be corrected to allow for fluctuations of the cosmological constant.

Calculating the the action for a general spherically symmetric static manifold without boundary where the cosmological constant is allowed to vary, one obtains

$$\begin{aligned} I &= -\pi r_-^2 - \pi r_+^2 - \int_{^{(3)}\mathcal{M}} \sigma \sqrt{^{(3)}g}\, d^3x - \alpha_j \int_{^{(3)}\mathcal{M}} n_j \sqrt{^{(3)}g}\, d^3x - \widehat{\rho_\Lambda} V_0^{(4)} \\ &= -S_{\text{bh}} - S_{\text{ch}} - S_{\text{matter}} - \alpha_j N_j - \widehat{\rho_\Lambda} V_0^{(4)}. \end{aligned} \tag{3.3.25}$$

If no black hole horizon exists, the first term in (3.3.25) is zero.

On the basis of (3.3.25), I see no reason to expect that spacetimes with low cosmological constant should dominate. Nor is it clear that the path integral will necessarily diverge if the four-volume is fixed and finite. To resolve these issues, however, is beyond the scope of this paper.

3.4 Summary

By virtue of the relation between the Euclidean action of a spacetime and its free energy, it is possible to conceive of quantum cosmology as as a generalized theory of statistical mechanics; the path integral being the partition function associated with a particular ensemble.

In order to set well defined problems, it is essential to know what thermodynamic quantities are to be held fixed in the partition function and which may be allowed to vary. From the first law derived in the previous two sections, it becomes clear what the relevant thermodynamic properties are–at least for spherically symmetric static spacetimes. With this information, it becomes possible to choose what set of conditions should be imposed on the physical system at hand.

Another compelling feature of the first law derived above, is that it reveals the compatibility of classical thermodynamic quantities and gravitational thermodynamic quantities. Traditionally, the conditions for gravitational thermal equilibrium have been considered distinct from the conditions for the thermal equilibrium of a matter distribution. It is usual to make a distinction between the thermal properties of a horizon and those of matter. However, from the above discussion it is clear that there is no need for such a formal distinction.

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CHAPTER 4

VARIATIONAL PRINCIPLES FOR NON–SMOOTH METRICS

4.1 Introduction

In[1] the Euclidean path integral approach to quantum gravity, the object of interest is a path integral of the form

$$Z = \int \mathcal{D}g_{\mu\nu} \exp\left[-I\left(g_{\mu\nu}\right)\right] \quad . \tag{4.1.1}$$

Here $g_{\mu\nu}$ is a Euclidean metric defined on a four-dimensional manifold $\mathcal{M}$, and $I\left(g_{\mu\nu}\right)$ is the Einstein action

$$I = -\frac{1}{16\pi}\int_{\mathcal{M}} d^4x\,(g)^{\frac{1}{2}}\,R \quad + \quad \text{boundary terms} \quad . \tag{4.1.2}$$

The boundary terms in (4.1.2) depend on $\mathcal{M}$ and on the boundary conditions imposed on the metric $g_{\mu\nu}$ [1,2]. One application of this path integral formalism is in black hole thermodynamics, where Z is interpreted as a thermodynamic partition function [2,3,4]. Another application is in quantum cosmology, where Z is interpreted as the wave function of the universe [5,6].

Much of the work with the path integral (4.1.1) has been done in the context of models where the four-metric is constrained to take a "spatially" homogeneous, (3 + 1) split form

$$ds^2 = N^2(t)dt^2 + h_{ij}\left(q^{\alpha}(t), \{\mathbf{x}\}\right)dx^i dx^j \tag{4.1.3}$$

[1]This is a version of a paper which was co-authored by Jorma Louko and will appear in *Physical Review D* (1990).

where $h_{ij}dx^i dx^j$ is the metric on a compact homogeneous three-manifold Σ, completely determined by the finitely many functions $q^\alpha(t)$. With this ansatz, the action takes the form

$$I = \int L(\dot{q}^\alpha, q^\alpha; N)\, dt \quad + \quad \text{boundary terms} \ . \tag{4.1.4}$$

Provided the ansatz is such that the Euler-Lagrange equations obtained from the Lagrangian in (4.1.4) are equivalent to the full Einstein equations for the ansatz, the issue of evaluating Z reduces to performing a quantum mechanical path integral of the form

$$Z = \int \mathcal{D}N(t)\mathcal{D}q^\alpha(t) \exp[-I] \ . \tag{4.1.5}$$

In which sense the minisuperspace integral (4.1.5) could be hoped to reflect the properties of the full path integral is largely an open question. For example, the paths $q^\alpha(t)$ contributing to (4.1.5) are expected to be continuous but nowhere differentiable in t, whereas the four-metrics $g_{\mu\nu}$ contributing to the full integral (4.1.1) would not be expected to be even continuous [7]. Nevertheless, there are problems in the formalism that are shared by the minisuperspace integral and the full integral, and it is often assumed that the minisuperspace integral gives a simple arena for studying such problems. A well known example is the issue of the contour of integration (see Ref. [8] and the references therein).

As the minisuperspace ansatz (4.1.3) is defined in terms of a $(3+1)$ decomposition of the metric, the minisuperspace path integral is directly applicable only for four-manifolds of the form $I \times \Sigma$, where the interval I may be either open, semi-open or closed. For example, if the interval is closed, the integral can be understood as a propagation amplitude between an "initial" and a "final" three-surface, on which the "initial" and "final" data could be chosen to be the intrinsic three-metrics, or the extrinsic curvature tensors, or some combinations thereof [1,9].

There are, however, physical situations which have prompted minisuperspace path integral constructions for manifolds which are not globally of the form $I \times \Sigma$. The case of particular interest, both from the viewpoints of black hole thermodynamics and quantum cosmology, is to take $\mathcal{M}$ to be compact with a single connected boundary [1,4,5,6]. In terms of the ansatz (4.1.3), one would then take the boundary to be the three-surface Σ_1 at (say) the upper limit of the coordinate time, $t = t_1$, and understand the lower limit $t = t_0$ as occurring at a coordinate singularity at the 'bottom' of $\mathcal{M}$. To construct the minisuperspace action in this case, one starts from the general Einstein action (4.1.2) defined on all of $\mathcal{M}$, imposes the symmetry dictated by the ansatz (4.1.3) in the region that is covered by the coordinate system of the ansatz, and derives the form of the minisuperspace action (4.1.4) paying careful attention to the coordinate singularity at $t = t_0$. One can then analyse the variational principle associated with the minisuperspace action and use general arguments of consistency to promote this minisuperspace variational principle into a minisuperspace path integral. Analyses of this kind have been given in Refs. [4,10,11].

An important ambiguity remains on the issue of what conditions to impose at the coordinate singularity at $t = t_0$. In the analyses of Refs. [4,10,11], one starts by considering metrics that are smooth on all of $\mathcal{M}$, in particular at $t = t_0$, and then passes to the minisuperspace action (4.1.4). At the level of the minisuperspace path integral (4.1.5), however, one can no longer expect to maintain smoothness in the initial conditions. This is because in a $(3+1)$ formulated path integral one expects to fix only a limited number of initial data at $t = t_0$, and this data should further be a quantum mechanically consistent set, in the sense of for example not attempting to fix simultaneously both a coordinate and its conjugate momentum. Some possibilities of consistently relaxing the initial conditions at the level of the minisuperspace action have been discussed in Ref. [11].

The purpose of this paper is to demonstrate, in a particular model, that one can relax the smoothness conditions at $t = t_0$ to allow conical or perhaps worse singularities already *before* passing to the minisuperspace action, and still recover a well defined variational principle. In particular, the variational principle yields smoothness of the extremizing metrics as an equation of motion. The classical solutions emerging from such a variational principle are thus smooth solutions to the Einstein equations on all of $\mathcal{M}$.

The question of how one might arrive at a well defined minisuperspace path integral from this kind of a variational principle, without explicitly appealing to smoothness in the initial conditions, will be left a subject of future work. We shall argue in Section 5, however, that the potential problems to be confronted in this approach are not obviously more severe than in the path integral constructions of Refs. [4,11].

A further interesting consequence of our work relates to the treatment of two dimensional singularities in general relativity, such as conical singularities associated with idealized cosmic strings. Motivated by the possibility of distributional matter sources in general relativity, Geroch and Traschen [12] have raised the question of how singular a metric can be in order to still have a Riemann tensor which is well defined in a distributional sense. They introduce a class of metrics, christened 'regular' metrics, which are less smooth than C^2 but satisfy conditions guaranteeing the existence of a distributionally well-defined Riemann tensor. They go on to prove that no metric in this 'regularity' class can have a source concentrated on a two dimensional hypersurface. However, the question of whether one might be able to arrive at a well defined action and variational principle associated with conically singular metrics was not resolved by their analysis since these metrics do not belong to their 'regularity' class. Here we show that, in fact, it is possible to define an action and a variational principle for at least some conically singular metrics.

We begin in Section 2, after a brief general discussion of singular configurations in a variational principle, by considering the more familiar variational problem for metrics which may have a jump discontinuity in the extrinsic curvature across a three-dimensional hypersurface. We exhibit the Einstein action for such metrics and demonstrate, in the absence of matter singularities, that the variational principle gives the absence of jump discontinuities as a 'generalized' Einstein equation. We also show how, in the presence of a singular matter distribution on a three-dimensional hypersurface, the standard junction conditions on this hypersurface [13] are directly obtained from the variational principle. Although these results have been anticipated in the earlier literature, especially in Refs. [2,14], they have not to our knowledge been previously explicitly stated.

In Section 3 we turn to the spatially homogeneous minisuperspace ansatz (4.1.3). We consider metrics defined on the manifold $\mathcal{M} = \bar{D} \times S^2$, where $\bar{D}$ is the closed two-dimensional disc, and we take these metrics to satisfy the ansatz (4.1.3) with $S^1 \times S^2$ spatial surfaces (known as the Kantowski-Sachs ansatz [15]). This is a situation of interest both in quantum cosmology and in black hole thermodynamics [3,4,11,16]. We assume that the metric is smooth everywhere on $\mathcal{M}$ except possibly at 'centre' S^2, which is not covered by the coordinate system of the ansatz. We then derive the minisuperspace action for these metrics, in the special case where the singularity at the centre is at worst conical. We demonstrate, in analogy with the extrinsic curvature discontinuities discussed in Section 2, that the minisuperspace variational principle gives the absence of a conical singularity as a generalized Einstein equation. In Section 4 we argue how a similar minisuperspace variational principle could be developed to incorporate a broader class of singularities than just conical ones.

The results are summarized and discussed in Section 5. We exhibit some of the as yet unresolved issues that would need to be confronted if one wishes to promote our non-smooth minisuperspace variational principles into genuine minisuperspace path integrals. We also comment on the relation of our minisuperspace variational principles to the question of Lorentzian versus Euclidean path integrals in quantum gravity.

4.2 Variational principle for discontinuities in the extrinsic curvature

A variational principle consists of an action functional whose stationary configurations subject to given boundary conditions are the solutions to the equations of motion subject to the same boundary conditions [17]. In classical mechanics and classical field theory, the equations of motion in general imply that the classical solutions will need to have certain regularity properties. When constructing an action principle, it is then usually sufficient to define an action functional on configurations that belong to the same regularity class as the classical solutions. For example, to derive Newton's equation for a particle in a one-dimensional smooth (say, C^1) potential $V(x)$, it is sufficient to consider the action

$$S([x];0,T) = \int_0^T dt \left(\tfrac{1}{2}m\dot{x}^2 - V(x)\right) \quad , \qquad (4.2.1)$$

on paths $x(t)$ belonging to the same smoothness class as the classical solutions.

However, it can occur that an action functional obtained in this way can be meaningfully extended to configurations that are considerably less smooth than the classical solutions. The question then arises as to whether the stationary configurations of the extended action are still the same as those of the original action.

For physically reasonable systems the answer would be expected to be positive. As a simple example, consider the action (4.2.1) with $V(x)$ (say) C^1. Suppose now that $x(t)$ is continuous for $0 \leq t \leq T$, and C^1 for $0 \leq t \leq T/2$ and $T/2 \leq t \leq T$. The action can then be expressed as the sum

$$S([x];0,T) = S([x];0,T/2) + S([x];T/2,T). \tag{4.2.2}$$

We wish to find the stationary configurations of this action subject to the boundary data $x(0) = x_0$, $x(T) = x_1$. For simplicity, vary the action first with respect to $x(t)$ on $0 < t < T/2$ and $T/2 < t < T$, with fixed $x(T/2) = y$, to obtain the ordinary equations of motion in the two regions. Then solve these equations and substitute back to the action to obtain

$$S(x_0, x_1; 0, T; y) = S_c(x_0, y; 0, T/2) + S_c(y, x_1; T/2, T) \tag{4.2.3}$$

where $S_c(x_0, y; 0, T/2)$ and $S_c(y, x_1; T/2, T)$ are the actions of the classical solutions with the indicated boundary data. The generic path in (4.2.3) will not solve the classical equations of motion at $t = T/2$, and it will indeed not even be C^1 there. However, extremizing (4.2.3) with respect to y yields the classical solution for the whole interval $0 \leq t \leq T$, and in particular yields the smoothness of the extremizing path at $t = T/2$ as an equation of motion. The reason is simply that by standard Hamilton–Jacobi theory $dS_c(x_0, y; 0, T/2)/dy$ is the momentum of the first half of the path at y and $dS_c(y, x; T/2, T)/dy$ is the negative of the momentum of the second half at y. This example is a special case of a discretization procedure which can be used to define path integrals for quantum mechanical systems with curved configuration spaces (see Ref. [18] and the references therein).

In general relativity, one similarly anticipates that an action functional appropriately extended to non-smooth metrics would still have its stationary configurations at the usual solutions to Einstein's equations. Here the situation is however considerably more complicated than in the example given above. Since the Ricci scalar is non-linear in the first derivatives of the metric, it becomes a very subtle question as to how singular a metric can be in order to still have a distributionally well-defined Riemann tensor and a well-defined action [12]. In this section we shall consider metrics that have at most a jump discontinuity in the extrinsic curvature at a three-dimensional hypersurface. For such metrics the Riemann tensor is well-defined as a distribution [12], but the jump discontinuities will give a non-vanishing contribution to the gravitational action. We shall demonstrate that when these contributions are properly taken into account, the situation is very similar to the example considered above.

Consider a general Euclidean line element in the ADM 3 + 1 formalism,

$$ds^2 = \left(N^2 + N_i N^i\right)dt^2 + 2N_i dt dx^i + h_{ij}dx^i dx^j, \qquad (4.2.4)$$

where N is the lapse function and N^i is the shift vector (latin indices extend from 1 to 3). Confine attention to spatially compact manifolds and take the Euclidean time coordinate, t, to extend from a 3-surface Σ_0 at $t = 0$ to a 3-surface Σ_1 at $t = 1$. We begin assuming that the metric is smooth (for concreteness, C^∞), and we shall relax this assumption later.

With the above representation, the four-curvature scalar density takes the form [19]

$$R\sqrt{g} = N\sqrt{h}\left(K^2 - K_{ij}K^{ij} +^{(3)} R\right) - 2\left(\sqrt{h}K\right)_{,0}$$

$$+ \quad 2(\sqrt{h}KN^i - \sqrt{h}h^{ij}N_{,j})_{,i}. \tag{4.2.5}$$

Here, K_{ij} is the extrinsic curvature tensor of a surface of constant t;

$$K_{ij} = \frac{1}{2N}\Big(\frac{\partial h_{ij}}{\partial t} - N_{i|j} - N_{j|i}\Big), \tag{4.2.6}$$

where a vertical bar indicates covariant differentiation with respect to h_{ij}. The gravitational scalar density (4.2.5) integrates to yield the Einstein Hilbert action,

$$I_{\text{E.H.}} = -\frac{1}{16\pi}\int R\sqrt{g}d^4x = \int_0^1 \mathcal{L}d^3x dt + \frac{1}{8\pi}\int_{\Sigma_1} K\sqrt{h}d^3x - \frac{1}{8\pi}\int_{\Sigma_0} K\sqrt{h}d^3x. \tag{4.2.7}$$

Here, $\mathcal{L}$ is a Lagrangian density first order in time derivatives,

$$\mathcal{L} = \frac{1}{16\pi}N\sqrt{h}\Big(K_{ij}K^{ij} - K^2 - {}^{(3)}R\Big). \tag{4.2.8}$$

In the Hamiltonian formulation, one defines a momentum conjugate to the 'field variable' h_{ij};

$$\pi^{ij} \equiv \frac{\partial\mathcal{L}}{\partial\dot{h}_{ij}} = \frac{1}{16\pi}\sqrt{h}\Big(K^{ij} - h^{ij}K\Big). \tag{4.2.9}$$

In this formulation, the Einstein–Hilbert action becomes

$$I_{\text{E.H.}} = \int\Big(\pi^{ij}\dot{h}_{ij} - N_i\mathcal{H}^i - N\mathcal{H}\Big)d^4x - \int_{\Sigma_1}\pi^{ij}h_{ij}d^3x + \int_{\Sigma_0}\pi^{ij}h_{ij}d^3x. \quad (4.2.10)$$

As first noticed by York [1], the Einstein-Hilbert action (4.2.10) is appropriate for a variational principle in which the values of π^{ij}, but not those of h_{ij} are fixed on Σ_0 and Σ_1. To obtain an action appropriate for fixing the canonical coordinates h_{ij} on Σ_0 and Σ_1, one must subtract a boundary term which cancels the boundary terms in (4.2.10). The resulting action is the York action [1,2]

$$I_{\text{Y}} = -\frac{1}{16\pi}\int_{\mathcal{M}} R\sqrt{g}d^4x - \frac{1}{8\pi}\int_{\partial\mathcal{M}} K\sqrt{h}d^3x. \tag{4.2.11}$$

Note, however, that these statements about the variational principle remain largely formal. In general, little is known about the existence of solutions to the classical boundary value problem with data fixed on Σ_0 and Σ_1. In the context of minisuperspace models, a discussion of this boundary value problem is given in [8].

We shall now relax the smoothness assumptions about the metric. Consider metrics which are regular everywhere on our manifold $\mathcal{M}$ except at a surface, Σ_τ, of constant time, $t = \tau$. We assume the intrinsic three metric h_{ij} to be continuous, but we allow the extrinsic curvature K_{ij} to have a finite discontinuity (jump discontinuity) at the surface Σ_τ. We need to evaluate the action for such metrics.

Break the time integral into three components

$$\begin{aligned} I &= -\frac{1}{16\pi}\left\{\left[\int_0^{\tau_-} + \int_{\tau_-}^{\tau_+} + \int_{\tau_+}^{1}\right]\int R\sqrt{g}d^3x dt\right\} + \text{ boundary terms} \\ &= I_1 + I_2 + I_3 + \text{ boundary terms}, \end{aligned} \tag{4.2.12}$$

where $\tau_\pm \equiv \lim_{\epsilon\to 0}\tau \pm \epsilon$. Since the metric is regular everywhere except at τ, actions I_1 and I_3 are well defined. For instance,

$$I_1 = \int_0^{\tau_-}\mathcal{L}d^3x dt + \frac{1}{8\pi}\int K\sqrt{h}d^3x\bigg|_{t=\tau_-} - \frac{1}{8\pi}\int K\sqrt{h}d^3x\bigg|_{t=0}. \tag{4.2.13}$$

Meanwhile for I_2 one has

$$\begin{aligned} I_2 &= \lim_{\epsilon\to 0}\left[\frac{1}{16\pi}\int_{\tau-\epsilon}^{\tau+\epsilon}\left[N\sqrt{h}\left(K_{ij}K^{ij} - K^2 - {}^{(3)}R\right)\right.\right. \\ &- \left.\left. 2\left(\sqrt{h}K\right)_{,0} + 2\left(\sqrt{h}KN^i - \sqrt{h}h^{ij}N_{,j}\right)_{,i}\right]d^3x dt\right]. \end{aligned} \tag{4.2.14}$$

In the first and third terms above, the worst irregularities are only jump discontinuities. So only the second term contributes,

$$I_2 = \frac{1}{8\pi}\int\left[K_+ - K_-\right]\sqrt{h}d^3x. \tag{4.2.15}$$

This is the contribution of the jump discontinuity to the action integral.

For definiteness, assume the York action (4.2.11). Substituting the expressions for I_1, I_2, and I_3, into equation (4.2.12) gives

$$I = \int_0^{\tau_-} \mathcal{L} d^3x dt + \int_{\tau_+}^1 \mathcal{L} d^3x dt. \tag{4.2.16}$$

This is the final form of our action, appropriate for metrics with a jump discontinuity in the extrinsic curvature on the surface Σ_τ. We shall now take the action (4.2.16) as the starting point of a variational principle and derive the corresponding equations of motion.

Under variation with respect to the metric components and their derivatives, the action functional (4.2.16) yields

$$\delta I_Y = \left\{ \int_0^{\tau_-} + \int_{\tau_+}^1 \right\} \left[\frac{\partial \mathcal{L}}{\partial g_{\mu\nu}} \delta g_{\mu\nu} + \frac{\partial \mathcal{L}}{\partial h_{ij,\mu}} \delta h_{ij,\mu} + \frac{\partial \mathcal{L}}{\partial h_{ij,kl}} \delta h_{ij,kl} \right] dt d^3x, \tag{4.2.17}$$

where greek indices range from 0 to 3 and latin range from 1 to 3. After integration by parts, this becomes,

$$\begin{aligned} \delta I_Y &= \frac{1}{8\pi} \int_0^{\tau_-} G^{\mu\nu} \delta g_{\mu\nu} \sqrt{g} d^4x + \frac{1}{8\pi} \int_{\tau_+}^1 G^{\mu\nu} \delta g_{\mu\nu} \sqrt{g} d^4x \\ &- \int_{\Sigma_0} \frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} \delta h_{ij} d^3x - \int \Big(\frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} \Big) \Big|_{\tau_-}^{\tau_+} \delta h_{ij} d^3x + \int_{\Sigma_1} \frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} \delta h_{ij} d^3x. \end{aligned} \tag{4.2.18}$$

It is vital to note that if the action is to be extremized under arbitrary variations $\delta g_{\mu\nu}$ for $0 < t < \tau_-$ and $\tau_+ < t < 1$ as well as arbitrary variations δh_{ij} at $t = \tau$, *each term in (4.2.18) must vanish independently.*

Recall that the York action (4.2.11) for smooth metrics is appropriate for keeping h_{ij} fixed on Σ_0 and Σ_1. We therefore wish also here to consider variations for which h_{ij} is fixed at these two boundaries but otherwise arbitrary. Requiring δI_Y (4.2.18) to vanish under such variations yields the usual Einstein equations

$$G^{\mu\nu} = 0 \tag{4.2.19}$$

for $0 < t < \tau$ and $\tau < t < 1$, whereas at $t = \tau$ we recover the equations

$$\frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}}\bigg|_{-}^{+} = \pi^{ij}\Big|_{-}^{+} = \left(K^{ij} - h^{ij}K\right)\Big|_{-}^{+} = 0. \tag{4.2.20}$$

Equations (4.2.20) are the well known surface Einstein equations for the 'vacuum' case [13].

The above treatment easily generalizes to account for the presence of matter. One starts from an action functional

$$I = I_{\text{grav.}} + I_{\text{matter}}. \tag{4.2.21}$$

By hypothesis, we take the matter to have a regular distribution everywhere except at $t = \tau$, where there is an infinitely dense, infinitely thin matter shell. Hence, the matter Lagrangian density is assumed to include a term of the form

$$\mathcal{L}_{\text{surf.}}\sqrt{h}\,\delta(t-\tau). \tag{4.2.22}$$

Define the intrinsic stress energy tensor of the surface by

$$S^{ij} = \frac{1}{\sqrt{h}}\frac{\partial}{\partial h_{ij}}\left(\mathcal{L}_{\text{surf.}}\sqrt{h}\right) \tag{4.2.23}$$

Then an extremization procedure analogous to the one performed above, yields the ordinary Einstein equations plus the surface Einstein equations in the presence of a matter shell [13],

$$\left(K^{ij} - h^{ij}K\right)\Big|_{\tau_-}^{\tau_+} = 8\pi S^{ij}. \tag{4.2.24}$$

The standard way to derive the surface Einstein equations is to assume that the ordinary Einstein equations are satisfied across a matter shell and then take the limiting case that the shell is infinitely thin. We have shown that they may be derived directly from the variational principle once the contribution of jump discontinuities in the extrinsic curvature have been included in the action.

Before leaving this discussion, it is appropriate to have a closer look at the boundary variations in (4.2.18). At both Σ_0 and Σ_1 extremization of the York action yields the condition

$$\frac{\partial \mathcal{L}}{\partial \dot{h}_{ij}} \delta h_{ij} = \pi^{ij} \delta h_{ij} = 0. \tag{4.2.25}$$

Clearly, setting $\delta h_{ij} = 0$ at the boundaries (*ie.* fixing the intrinsic 3-metric there) is sufficient to guarantee that the boundary variations are zero. However, one can imagine physical situations where the intrinsic 3-metric is not fixed on the boundary. This would be the gravitational version of 'natural boundary conditions' in the variational problem. A familiar example of such natural boundary conditions is a flag whose end is allowed to fly freely in the breeze [20]; another example is provided by the open relativistic string [21]. If now arbitrary variations of h_{ij} are allowed at a boundary then a condition for extremizing the gravitational action is

$$\pi^{ij} = \sqrt{h}\left(K^{ij} - h^{ij} K\right) = 0 \tag{4.2.26}$$

at the boundary where h_{ij} is not fixed. This means that not fixing h_{ij} at a boundary forces the extrinsic curvature to vanish there. It might be of interest to study whether such 'natural boundary conditions' would be relevant for path integral constructions in the context of quantum cosmology and black hole thermodynamics.

4.3 Kantowski-Sachs ansatz on $\bar{D} \times S^2$ with conical singularities

We shall now consider metrics defined on the manifold $\mathcal{M} = \bar{D} \times S^2$, where $\bar{D}$ is the closed two-dimensional disc. We take the metrics to obey the Kantowski-Sachs ansatz [15]

$$ds^2 = N^2(t)dt^2 + a^2(t)dz^2 + b^2(t)d\Omega_2^2, \tag{4.3.1}$$

where z is periodic with period 2π and $d\Omega_2^2$ is the line element for the unit 2-sphere. The Euclidean time coordinate t is interpreted as the radial coordinate on the disc. We assume the metrics to be smooth (for concreteness, C^∞) everywhere on $\mathcal{M}$ except possibly at the 'centre' S^2, which is not covered by the coordinate system of the ansatz. Further, we assume the possible singularities at the centre to be so mild that $\int_{\mathcal{M}} d^4x\, (g)^{\frac{1}{2}} R$, and hence the Einstein action, is still well-defined.

We shall consider the York action (4.2.11), which is appropriate for fixing the intrinsic three-metric on the boundary $\partial\mathcal{M}$. This is directly the action relevant for the no-boundary proposal in quantum cosmology [5,6]. In black hole thermodynamics, one would usually consider an action with the additional boundary term

$$+\frac{1}{8\pi}\int_{\partial\mathcal{M}} d^3x\, (h)^{\frac{1}{2}} K_0 \tag{4.3.2}$$

which normalizes the action and the black hole energy to agree with the conventional results in asymptotically flat space [2,3,14]. This boundary term is, however, a function of the intrinsic boundary three-metric only, and its presence will therefore not affect our discussion of the variational principle with fixed boundary three-metric.

We need to evaluate the action (4.2.11) for our metrics and to examine the resulting variational principle. Without loss of generality, we can take $t = 0$ to correspond to the S^2 'centre' of $\mathcal{M}$, and $t = 1$ to correspond to the three-surface Σ_1 at $\partial\mathcal{M}$. For $0 < t \leq 1$, the coordinate system of the ansatz is regular, and we can insert the ansatz into (4.2.11), integrate over the three-surfaces, and perform a standard integration by parts to eliminate the second time derivatives [22]. The action can thus be written as

$$I = \lim_{\epsilon\to 0_+}\left\{2\pi\int_\epsilon^1 L\,dt - \frac{\pi}{N}\frac{d}{dt}\left(ab^2\right)\bigg|_{t=\epsilon}\right.$$

$$-\frac{1}{16\pi}\int_{t<\epsilon} d^4x\,(g)^{\frac{1}{2}}\,R\Big\} \qquad (4.3.3)$$

where the Lagrangian L is given by

$$L = \frac{N}{2}\left(-\frac{a\dot{b}^2 + 2b\dot{a}\dot{b}}{N^2} - a\right) \ . \qquad (4.3.4)$$

Let us first recall what happens if we take the metrics to be smooth on all of $\mathcal{M}$ [4,10,11,16]. In this case the functions $a(t)$, $b(t)$ and $N(t)$ must at $t \rightarrow 0$ satisfy the conditions

$$\begin{aligned} a(t) &\longrightarrow 0 \\ \frac{\dot{b}(t)}{N(t)} &\longrightarrow 0 \\ \frac{\dot{a}(t)}{N(t)} &\longrightarrow 1 \end{aligned} \qquad (4.3.5)$$

as well as further conditions on the higher t-derivatives. Also, the last term in (4.3.3) will vanish. Using (4.3.5), the action can be written as

$$I = 2\pi\int_0^1 L\,dt \quad - \quad \pi b^2\Big|_{t=0} \qquad (4.3.6)$$

where the quantities at $t = 0$ are understood as limits as $t \rightarrow 0$.

When interpreting this action, it is important to bear in mind that the coordinate singularity at $t = 0$ is not a boundary of $\mathcal{M}$. So while the term $-\pi b^2|_{t=0}$ in (4.3.6) may resemble a 'boundary term', it, in fact, is not. We now coin the expression "limit term" which will refer to terms in the $(3+1)$ decomposed action and its variation which are evaluated either at $t = 0$ or at the boundary at $t = 1$.

Varying the action (4.3.6) yields

$$\delta I \;=\; 2\pi\int_0^1 dt\left(\frac{\delta L}{\delta a}\,\delta a + \frac{\delta L}{\delta b}\,\delta b + \frac{\partial L}{\partial N}\,\delta N\right)$$

$$-\pi \frac{\dot{a}}{N} \delta\left(b^2\right)\Big|_{t=1} - 2\pi \frac{\dot{b}}{N} \delta(ab)\Big|_{t=1}$$
$$+\pi \left(\frac{\dot{a}}{N} - 1\right) \delta\left(b^2\right)\Big|_{t=0} + 2\pi \frac{\dot{b}}{N} \delta(ab)\Big|_{t=0} \tag{4.3.7}$$

where $\delta L/\delta a$ and $\delta L/\delta b$ are the usual Euler-Lagrange variational derivatives,

$$\frac{\delta L}{\delta q} = \frac{\partial L}{\partial q} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) \quad . \tag{4.3.8}$$

The limit terms at $t = 0$ in (4.3.7) vanish by virtue of the assumption of smoothness, as is seen from (4.3.5). If the boundary three-metric is taken to be fixed, the limit terms at $t = 1$ vanish as well. Extremization of the action in this class of metrics therefore gives the standard Einstein equations

$$0 = \frac{\delta L}{\delta a} = \frac{\delta L}{\delta b} = \frac{\partial L}{\partial N} \tag{4.3.9}$$

for $t > 0$, and our regularity assumptions guarantee that the solutions to (4.3.9) can be extended to smooth solutions on all of $\mathcal{M}$. We therefore see that the minisuperspace action (4.3.6), together with the regularity assumptions at $t \to 0$, gives a minisuperspace variational principle appropriate for the manifold $\mathcal{M}$ with the intrinsic three-metric fixed on $\partial\mathcal{M}$. The classical solutions are well known to be part of the Euclidean Schwarzschild solution, with mass determined by the values of the boundary scale factors [3,11,16].

Two points here should be emphasized. Firstly, although the action (4.3.6) was written in a $(3+1)$ form, the boundary conditions for the metrics have been specified in an intrinsically four-dimensional way. In particular, the assumption of four-dimensional smoothness at the coordinate singularity at $t = 0$ implies all the conditions (4.3.5), as well as further conditions for the higher t-derivatives. No question of counting 'independent' pieces of initial data has arisen. This question would only arise at the next step, when attempting to give a $(3+1)$ formulated variational principle with initial data that could be used in a minisuperspace path integral of the form (4.1.5) [10,11].

Secondly, the limit term at $t = 0$ in the action (4.3.6) could have been written in a number of different forms which are all equivalent under the assumption of smoothness. For example, the term could have been written as

$$-\frac{\pi}{N}\frac{d}{dt}\left(ab^2\right)\bigg|_{t=0} \quad . \tag{4.3.10}$$

Depending what form is chosen for this term, the limit terms at $t = 0$ in δI can take a number of superficially different forms, which nevertheless are all equivalent and vanishing under the smoothness assumptions. Again, the question of choosing between the different forms of the limit term in (4.3.6) would only arise at the level of a $(3+1)$ formulated variational principle [11].

We now turn to metrics which are not necessarily smooth at the centre of $\mathcal{M}$. For such metrics the conditions (4.3.5) need not necessarily hold, nor need the last term in the action (4.3.3),

$$\lim_{\epsilon\to 0_+}\left[-\frac{1}{16\pi}\int_{t<\epsilon} d^4x\,(g)^{\frac{1}{2}}\,R\right] \quad , \tag{4.3.11}$$

necessarily vanish. We wish to evaluate (4.3.11) for such metrics and find the corresponding minisuperspace variational principle.

In the rest of this section we shall assume that the singularity at $t \to 0$ is at worst conical. More precisely, we assume that the metric can be written as

$$ds^2 = F^2\left(dx^2 + dy^2\right) + b^2 d\Omega_2^2 \tag{4.3.12}$$

where

$$F^2(x,y) = \left(x^2+y^2\right)^{-\alpha} f(x,y) \quad , \tag{4.3.13}$$

as $t \to 0$, as well as further conditions on the higher time derivatives. Using these conditions and the result (4.3.14), we now see that the minisuperspace action (4.3.3) takes a form identical to (4.3.6). The quantities at $t = 0$ are again understood as limits as $t \to 0$.

Let us now vary the minisuperspace action (4.3.6), keeping fixed the values of a and b at the boundary $t = 1$, requiring the variables to obey the conical singularity conditions as $t \to 0$, but not fixing the actual value of the deficit angle at the conical singularity. The variation is again given by (4.3.7). Recall that if the action is to be extremized under arbitrary variations, each term in (4.3.7) must vanish independently. The limit terms at $t = 1$ again vanish by the assumption of fixing the boundary values of a and b. Similarly, the second limit term at $t = 0$ vanishes by the equations (4.3.16) which are implied by our conical singularity assumptions. However, the first limit term at $t = 0$ is not identically vanishing, since the conical singularity conditions (with unspecified deficit angle) do not fix the limiting values of b and $\dot{a}/N$ as $t \to 0$.

Requiring that the action be stationary under arbitrary variations δa, δb and δN satisfying our boundary conditions, we now obtain the usual Einstein equations (4.3.9) for $t > 0$, as well as the equation

$$\left.\frac{\dot{a}}{N}\right|_{t=0} = 1 \quad . \tag{4.3.18}$$

Taken together with the conical singularity conditions we imposed at $t = 0$, the condition (4.3.18) guarantees that the solutions to the Einstein equations (4.3.9) for $t > 0$ can be extended to smooth solutions of the Einstein equations over all of $\mathcal{M}$. These solutions are the same Euclidean Schwarzschild solutions that are recovered from the variational principle in which one initially restricts the variations to smooth metrics on all of $\mathcal{M}$. The difference between the two variational principles is only in the class of the metrics included in the variations: with our conical singularity conditions the smoothness at $t = 0$ is not put in as an assumption, but it emerges from varying the action as an equation of motion.

In the above discussion we have understood the conical singularity conditions at $t \to 0$ to be those following from the metric (4.3.12–4.3.13). We now note that the conditions in the minisuperspace variational principle at $t = 0$ can in fact be relaxed to consist only of the set (4.3.16). For consider the action (4.3.6) as defined on functions of t, assuming only that a, b, $\dot{a}/N$ and $\dot{b}/N$ have finite limits as $t \to 0$ and that the conditions (4.3.16) are satisfied. The variation of the action is again given by (4.3.7). Requiring that the action be stationary under variations for which a and b are fixed at $t = 1$ gives again the Einstein equations (4.3.9) for $t > 0$ and the condition (4.3.18) at $t = 0$. Combined with (4.3.16), this is sufficient to guarantee that the classical solutions are extendible to smooth solutions of the Einstein equations on all of $\mathcal{M}$.

We summarize. The action (4.3.6), defined on smooth functions of $t \in (0, 1]$ such that a, b, $\dot{a}/N$ and $\dot{b}/N$ have finite limits as $t \to 0$, subject to the conditions

$$a, b \quad \text{fixed at } t = 1 \ , \tag{4.3.19}$$

$$a = 0 \ , \ \frac{\dot{b}}{N} = 0 \quad \text{at } t = 0 \ , \tag{4.3.20}$$

gives a minisuperspace variational principle whose extremizing metrics are smooth solutions to the Einstein equations on $\mathcal{M}$. The conditions (4.3.20), with the Einstein equations for $t > 0$, do not by themselves guarantee smoothness of the solutions on all of $\mathcal{M}$. However, variation of the action gives, in addition to the usual Einstein equations for $t > 0$, one more condition (4.3.18) as $t \to 0$, and this will be sufficient to guarantee smoothness of the solutions on all of $\mathcal{M}$.

It is worth noting that this variational principle is to some extent analogous to the 'natural boundary conditions' discussed at the end of Section 2. In both cases the variation of the action contains, in addition to the integrals of the usual Euler-Lagrange terms, also a limit term. A variation of this kind is nevertheless well defined. The situation is similar with the more familiar variational principles for a flag whose end is allowed to fly freely [20] and for the open relativistic string [21].

4.4 Kantowski-Sachs ansatz on $\bar{D} \times S^2$: more general singularities?

In the previous section we restricted the singularities in the Kantowski-Sachs metric at the centre of $\mathcal{M}$ to be at worst conical. For discussing variational principles based on the Einstein action this restriction is unnecessarily strong, since one only needs the singularity to be so mild that $\int_{\mathcal{M}} d^4x\, (g)^{\frac{1}{2}}\, R$ is still well defined. For example, in (4.3.12) the smoothness conditions for $b(x,y)$ at $x = y = 0$ could be to some extent relaxed.

It might be a problem of interest to give an exhaustive classification of the sufficiently mild singularities and the corresponding variational principles with the Kantowski-Sachs ansatz on $\bar{D} \times S^2$. It might also be of interest to investigate whether such singularities could in some sense be understood as limiting cases of metrics that have a jump discontinuity in the extrinsic curvature at a three-surface of constant t.

With a conical singularity metric, a limiting procedure of this kind can be given as follows. For a given number ϵ satisfying $0 < \epsilon < 1$, consider a continuous metric g_ϵ which coincides with the prescribed conical singularity metric for $t \geq \epsilon$, has a jump discontinuity in the extrinsic curvature at the surface $t = \epsilon$, and is smooth for $t \leq \epsilon$ with $b(t) = b(\epsilon)$ and $a(t) = \int_0^t N(t')dt'$. At the limit $\epsilon \to 0$, the action of g_ϵ is easily seen to approach the action of the prescribed conical singularity metric. In particular, the contribution (4.3.11) from the conical singularity is obtained as the limit $\epsilon \to 0$ of the contribution from the surface $t = \epsilon$,

$$\frac{1}{8\pi} \int_{t=\epsilon} \Big(K_+ - K_-\Big) \sqrt{h}\, d^3x$$

$$= \frac{\pi}{N} \frac{d}{dt} \left(ab^2\right)\Big|_{t=\epsilon_+} - \frac{\pi}{N} \frac{d}{dt} \left(ab^2\right)\Big|_{t=\epsilon_-} , \qquad (4.4.1)$$

where K_- and K_+ are the limiting forms of the extrinsic curvature scalar on the surface $t = \epsilon$ when approaching this surface respectively from $t < \epsilon$ and $t > \epsilon$. If an analogous limiting procedure can be justified for singularities worse than conical, comparison of (4.3.3) and (4.4.1) suggests that our action (4.3.6) may be the appropriate minisuperspace action also for more general singularities than just conical ones.

We shall not attempt to develop the above ideas to a more precise level. Recall that in Section 3 we first introduced the minisuperspace variational principle with conical singularities in a formulation where the conical singularity conditions were given in terms of the four-dimensional metric (4.3.12). These conical singularity conditions included, but were not restricted to, the conditions (4.3.16). In the end, however, we were able to give a minisuperspace variational principle with weaker initial conditions consisting just of (4.3.16). For analysing the consistency of the minisuperspace variational principle in its own right, there was no need to establish a direct connection between the full action (4.2.11) and the minisuperspace action (4.3.6) under the weaker initial conditions (4.3.16): it was sufficient to notice that these actions coincided for the classical solutions that came out of the minisuperspace variational principle. We shall therefore not attempt to give a four-dimensional analysis of singularities more general than conical. Rather, motivated by the considerations in the previous paragraph, we shall now just start from the minisuperspace action (4.3.6), and investigate the variational principle given by this action when the initial conditions used in Section 3 for the functions $a(t)$, $b(t)$ and $N(t)$ are relaxed.

Consider thus the minisuperspace action (4.3.6) defined on functions of t such that a, b, $\dot{a}/N$ and $\dot{b}/N$ have finite limits as $t \to 0$, but the values of these limits are not specified. The variation of this action is again given by (4.3.7). Requiring the action to be stationary under variations which keep a and b fixed at $t = 1$, we recover now the standard Einstein equations (4.3.9) for $t > 0$, as well as the conditions

$$\begin{aligned} \left.\frac{\dot{a}}{N}\right|_{t=0} &= 1 \\ \left.\frac{\dot{b}}{N}\right|_{t=0} &= 0 \ . \end{aligned} \tag{4.4.2}$$

It is straightforward to verify that the conditions (4.4.2), combined to the Einstein equations for $t > 0$, are indeed sufficient to guarantee that the classical solutions can be extended to smooth solutions on all of $\mathcal{M}$.

We have thus shown that the action (4.3.6) gives a minisuperspace variational principle appropriate for solutions defined on all of $\mathcal{M}$, even when the boundary conditions in the variational principle only consist of specifying the final values of a and b at $t = 1$ but 'nothing' at $t = 0$. The conditions at $t = 0$ that are necessary to make the solutions extendible to all of $\mathcal{M}$ will themselves come out of the variational principle as equations of motion. One might regard this minisuperspace variational principle as being the one most closely analogous to the variational principle appropriate for the manifold $\mathcal{M}$ in the full theory.

4.5 Discussion

In this paper we have analysed the variational principle of general relativity for two classes of metrics that are not necessarily smooth but for which the Einstein action can still be defined in a unambiguous way. These were metrics with 1) a jump discontinuity in the extrinsic curvature at a three-dimensional hypersurface, and 2) a conical singularity occurring in Euclidean Kantowski-Sachs metrics on the manifold $\bar{D} \times S^2$. In both cases we demonstrated that the vacuum variational principle gives, in addition to the usual Einstein equations, the smoothness of the extremizing metrics as part of the equations of motion. This means that the classical solutions are the same smooth metrics that would be obtained when the variational principle is initially defined only for smooth metrics. With the former class of metrics, we also showed that in the presence of a singular matter distribution on a three-dimensional hypersurface the usual junction conditions on this hypersurface are directly recovered from our variational principle as equations of motion.

At the purely classical level, our variational principles do not contain anything surprising. A variational principle in general relativity consists of an action functional whose stationary configurations subject to given boundary conditions are the solutions to the Einstein equations subject to the same boundary conditions. In the vacuum theory the classical solutions of interest are smooth metrics, and in the classical variational principle it is then sufficient to take also the neighbouring, non-classical metrics to be smooth. If the action functional obtained in this way can be extended also to non-smooth metrics, such that neither the four-manifold on which the metrics live nor the boundary conditions for these metrics are changed, it is then expected that the stationary configurations of the extended action be still those of the old action: the extended variational principle should give the smoothness of the extremizing metrics as 'generalized' Einstein equations. Similarly, if we introduce matter with a singular Lagrangian but a well-defined action, a carefully defined total action would be expected to lead to the appropriate 'generalized' Einstein equations at the singular matter source, provided these equations exist in some suitable distributional sense [12]. The variational principles presented in this paper are just special cases of this construction, under specific choices for the potential singularities.

Our minisuperspace variational principles become more interesting when viewed as a starting point for constructing a minisuperspace path integral. A path integral must in general be defined by a careful regularization procedure, and the contributing paths will usually not be smooth even when the classical variational principle is initially defined for smooth paths. For example, the paths $q^\alpha(t)$ contributing to a quantum mechanical path integral of the type (4.1.5) are expected to be continuous but nowhere differentiable in t. When we now wish to understand a minisuperspace path integral of the type (4.1.5) as a sum over metrics on a manifold which does not admit a global (3+1) decomposition, the smoothness of the metrics becomes an issue already one step before the actual regularization of the integral in (4.1.5), namely, at the stage of choosing the end-point conditions in this integral at the upper and lower limits of t. As the quantum mechanical end-point conditions should be consistent with the boundary conditions of the classical variational principle, it is thus of importance to choose the classical minisuperspace variational principle to correspond to an appropriate smoothness class of metrics. The choice of this appropriate smoothness class would, in the end, have to be justified by establishing a connection between the minisuperspace path integral and the path integral of the full theory.

With Kantowski-Sachs metrics on the manifold $\mathcal{M} = \bar{D} \times S^2$, we showed explicitly how the choice of the smoothness assumptions at the 'centre' of $\mathcal{M}$ is reflected in the 'initial' conditions of the minisuperspace variational principle. Our analysis thus complements those given in Refs. [4,10,11], where the metrics in the variational principle were first taken to be smooth on all of $\mathcal{M}$ and the smoothness conditions were relaxed only at the level of the minisuperspace action.

To follow Refs. [4,11] and to promote our minisuperspace variational principles into genuine path integrals, one would need to give a detailed definition of the path measure, including a specification of a convergent contour of integration. We shall not attempt to embark on this task here, but we would nevertheless like to end by briefly discussing some issues that could arise in this context.

For definiteness, consider the variational principle presented in Section 4: the action is given by (4.3.6), and the fixed quantities in the variational principle are the values of a and b at $t = 1$ but 'nothing' at $t = 0$. The first question in the path integral would then be how to implement the initial 'nothing.' One way to proceed is to notice from the limit term in (4.3.7) that the action (4.3.6) gives a generically well-defined variational principle for metrics on the manifold $[0, 1] \times S^1 \times S^2$, provided the fixed quantities both at $t = 0$ and $t = 1$ are the values of a and b. It should therefore be possible to construct with this action a path integral between fixed initial a_0, b_0 and final a_1, b_1. The path integral for $\bar{D} \times S^2$, fixing 'nothing' at the centre, could then be obtained by integrating over all choices of the initial data,

$$Z(a_1, b_1) = \int \mu \, da_0 \, db_0 \int_{a_0, b_0}^{a_1, b_1} \mathcal{D}N \, \mathcal{D}a \mathcal{D}b \exp[-I] \quad , \tag{4.5.1}$$

where μ could be chosen to depend on a_0 and b_0. To proceed from here, there are at least two different routes. One could start by defining first the $\mathcal{D}N\mathcal{D}a\mathcal{D}b$

path integral on the right hand side of (4.5.1), and only after that address the two ordinary integrals over a_0 and b_0. The ordinary integrals would then formally amount to a (generalized) Laplace-Fourier transform [23]. Alternatively, one could first take one or both of the ordinary integrals under the path integral, for example by giving an explicit discretization, and address the definition of the path integral only after that. One would perhaps hope that either method should in the end lead to the same answer; however, to substantiate this hope one would need to give precise definitions of each of the respective path integrals, including the contours of integration. One would in particular need to specify the contours for the Laplace-Fourier transformations in a way compatible with the contours for the path integrals.

Finally, we note that our minisuperspace variational principles and path integrals, especially (4.5.1), bear a superficial similarity to path integrals that have been advocated by a number of workers from purely Lorentzian considerations [9,24]. It should be emphasized that our starting point in the minisuperspace analysis was essentially topological: the manifold $\mathcal{M} = \bar{D} \times S^2$. Although we formulated the variational problem in the Euclidean signature, we can relax this by taking the functions $a(t)$, $b(t)$ and $N(t)$ to be complex-valued. In fact, in the classical boundary value problem the signature of the solutions cannot be specified as part of the problem, but the signature will come out as part of the solution. For certain (real) values of the boundary scale factors the only solutions to our boundary value problem are indeed neither Euclidean nor Lorentzian but genuinely complex-valued metrics [3,11,16]. To what extent the resulting path integrals, such as (4.5.1), can be thought of as being Lorentzian, falls then under the question of specifying the contour of integration. With path integrals constructed from a minisuperspace action initially defined for metrics that are smooth on all of $\mathcal{M}$, this question has been discussed in Ref. [11].

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CHAPTER 5

BLACK HOLES WITH POSITIVE HEAT CAPACITY

A[1] recent paper by Balbinot and Barletta [1] raises the interesting possibility that stable, non-evaporating mini-black holes with masses several times the Planck mass may be the end product of the evaporation process. They show that zero-temperature static black hole states will exist if the vacuum polarization at the horizon is dominated by fields (vector bosons) whose energy density there is positive. This very important observation has obvious implications for the dark matter problem in cosmology.

However, a point which should not be minimized is that the horizon energy density due to vacuum polarization depends critically on the nature of the black hole's time evolution. It becomes a question of importance whether the *static* black hole states of Balbinot and Barletta can actually be reached by *dynamic* evolution of an evaporating black hole.

Detailed information about the vacuum stress tensor is currently available for static ("Hartle-Hawking") black holes and, in this case, the vacuum energy density at the horizon may be positive for vector boson fields [2]. However, nothing is known presently about the sign of the energy density for the "Unruh" vacuum appropriate for an evaporating black hole. As Elster has pointed out, one would expect that the horizon energy density in the Unruh vacuum to be less than for the Hartle-Hawking vacuum because in the case of the Unruh vacuum there will be no (positive) contribution to the horizon energy density from incoming thermal

[1] A version of this paper has been published:
G. Hayward, "Black Holes with positive specific heat," *Classical and Quantum Gravity* 6 *(1989) L25.*

radiation. Hence, it may well be that the horizon energy density for an evaporating black hole is negative; in which case, rather than stop evaporating, the black hole would actually evaporate much more rapidly in final stages.

Although we are not in a position to resolve the fate of an evaporating black hole, Balbinot and Barletta's observation may still have important physical consequences.

We confine our attention to a static spherically symmetric black hole with the general line element,

$$ds^2 = -\left(1 - \frac{2m(r)}{r}\right) e^{2\psi(r)}dv^2 + e^{\psi(r)}drdv + r^2 d\Omega^2. \tag{5.1}$$

where ψ and m are functions of the radial coordinate r. By a coordinate transformation,

$$dt = dv - \frac{dr}{(1 - \frac{2m}{r})}, \tag{5.2}$$

we obtain the more familiar form,

$$ds^2 = e^{\psi}\left(-f(r)dt^2 + \frac{dr^2}{f(r)}\right) + r^2 + d\Omega^2 \tag{5.3}$$

where $f(r) = (1 - \frac{2m(r)}{r})e^{\psi}$.

Following Bardeen's example [3], we define the mass of the black hole as $M = m(r)|_{r=2m}$. Also, we let $r_0 = 2M$. The surface gravity is then

$$\begin{aligned} \kappa &= \frac{1}{2}f'(r)\Big|_{r=r_0} \\ &= \frac{1}{2}e^{\psi(r)}\left(\frac{2M}{r^2} - 4\pi r^2\rho(r)\right)\Big|_{r=r_0} \end{aligned} \tag{5.4}$$

where it is understood that $\psi(\infty) = 0$.

The usual way to define the Hawking temperature is to impose the condition of periodicity in Euclidean time. For a Schwarzschild black hole we obtain for the temperature measured by a stationary observer at radius R

$$\begin{aligned} T &= \frac{\kappa}{2\pi}\left(g_{00}(R)\right)^{-1/2} \\ &= \frac{1}{8\pi M}\left(g_{00}(R)\right)^{-1/2}, \end{aligned}$$

where setting $R = \infty$ gives the classic result $T = \frac{1}{8\pi M}$.

Directly applying this condition of periodicity in Euclidean time to the metric in equation (5.1) yields,

$$T(R) = \frac{e^{\psi(r)-\psi(R)}}{2\pi\left(1-\frac{2m}{R}\right)^{1/2}}\left(\frac{2M}{r^2} - 4\pi r^2\rho(r)\right)\Bigg|_{r=r_0} . \tag{5.5}$$

Evaluating at $R = \infty$ yields

$$T = e^{\psi(r)}\left(\frac{M}{2\pi r^2} - 2r\rho(r)\right)\Bigg|_{r=r_0} . \tag{5.6}$$

This is the expression for black hole temperature used by Balbinot and Barletta.

To avoid unnecessary complications due to global geometric effects, we consider the idealized case of a black hole enclosed in a tight-fitting perfectly reflecting sphere of radius R_0. We then imagine the space outside the spherical shell to be devoid of radiation so that $\rho(r) = 0$ for $r > R_0$. R_0 should be small enough so that the geometry closely approximates a Schwarzschild manifold and we can set $\psi(r) = \text{constant} = 0$. On the other hand, we must pick R_0 large enough so that boundary effects on the energy density within the sphere are negligible. A result due to Elster [2] indicates that, at least for vector boson fields a sphere radius of $R_0 \geq 3M$ is ample. We now imagine that a distant observer measures temperature by means of a heat-conducting filament connecting him to the black hole.

This formal model allows us to isolate the thermodynamic quantities in the vicinity of the black hole and transform them according to what would be detected by a distant observer in the absence of intervening radiation.

The temperature observed at infinity with this model, for which we may set $\psi(r) = 0$, is

$$T = \left(\frac{1}{8\pi M} - 4M\rho(r_0)\right). \tag{5.7}$$

From both equation (5.5) and equation (5.7), it is clear that as the energy density on the horizon approaches $\frac{1}{32\pi M^2}$, the black hole approaches zero temperature. Elster has shown [2] that for a black hole enclosed in a spherical reflecting shell such as we have proposed, the energy density on the horizon due to vacuum polarization is

$$\rho_{vac.} = \frac{41N}{7680\pi^2 M^4}$$

where N is the number of vector boson fields. Substituting into equation (5.7), we see that the black hole approaches zero temperature as

$$M \to \left(\frac{41N}{240\pi}\right)^{1/2}.$$

This result is meaningful only if N is large enough that we may safely ignore quantum gravitational effects. In supersymmetric string theory, for instance, $N = 496$. With this value, the zero temperature limit occurs when $M \approx 5M_{\text{pl.}}$ which we take to be large enough to be beyond the quantum gravitational regime.

We now seek to derive an expression for the the heat capacity of the black hole. It is most convenient to derive the heat capacity in terms of the temperature, T, and the total energy, M, of the black hole as defined from infinity. We then have,

$$\frac{\partial T}{\partial M} = \left(-\frac{1}{4M^2} + \frac{41N}{320\pi M^4}\right). \tag{5.8}$$

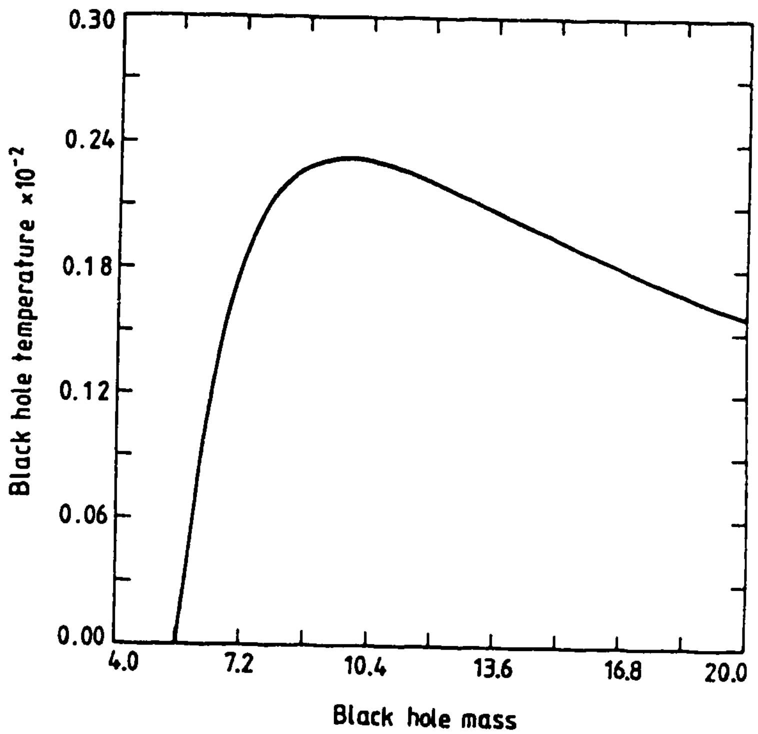

Figure 5.1: Graph of temperature against mass with $N = 500$ for a black hole enclosed in a tight–fitting spherical shell.

Interestingly enough, we find $\frac{\partial T}{\partial M}$, is positive for black holes in the mass range

$$\left(\frac{41N}{240\pi}\right)^{1/2} < M < \left(\frac{41N}{80\pi}\right)^{1/2}. \tag{5.9}$$

With N given by supersymmetric string theory, this corresponds to a mass range between $5M_{\text{pl.}}$ and $9M_{\text{pl.}}$ (see Figure 5.1).

Unlike classical black holes which have negative heat capacity, black holes in this mass range should in principle be able to maintain equilibrium with surrounding radiation under adiabatically changing boundary conditions (ie. conditions which approximate a slowly changing Hartle-Hawking state).

It is important to note that the positive heat capacity result in expression (5.9) depends on the boundary conditions we have imposed only in as much as these conditions allow us to isolate the heat capacity of the black hole from contributions of the energy distribution external to the black hole.

What role these black hole solutions with positive heat capacity might play in a cosmological model remains an open question. It is interesting to speculate that that primordial black holes may have formed in the early universe in a state approximating the Hartle-Hawking vacuum. Those that were in such a mass range as to have positive heat capacity may have been able to maintain thermodynamic equilibrium with the cooling Universe and so may still persist at near zero temperature and at a finite mass:

$$M \approx \left(\frac{41N}{240\pi}\right)^{1/2}. \tag{5.10}$$

Even though the initial density of such black holes may have been quite small, their relative contribution to the cosmological density would increase proportionately to the scale factor $a(t)$. Indeed, MacGibbon [4] has argued that stable relics of primordial black holes of a few Planck masses could make an important contribution to the current density of the Universe, possibly even large enough to provide the critical density.

We have argued that Balbinot's claim that conventional black holes may stop radiating somewhere above the planck mass is not yet justified by the available evidence. Further, we have shown the existence of positive heat capacity black hole solutions. What role such solutions may actually play in cosmology is a subject for future research[2].

[2] *Addendum.* The result of this letter should hold for any situation in which the energy density on the horizon is positive, for instance, if massive Higgs fields and massive boson fields contribute significantly to the horizon energy density. In this letter we have suggested, based on a result

by Elster [2], that the energy density on the horizon due to massless Abelian boson fields is also positive. This result has recently been placed in doubt by a Jensen and Ottewill (Oxford University Preprint, 1988).

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CHAPTER 6

BLACK HOLES IN THE EARLY UNIVERSE

6.1 Introduction

Since [1] Zel'dovich [1] and Hawking [2] postulated the existence of primordial black holes (PBH's), there has been considerable interest in determining what cosmological significance they might have. PBH's have been considered as a factor in a broad assortment of cosmological problems ranging from baryogenesis [3], to the missing mass problem [4], to galactic nucleation [5]. Classically, PBH's form due to density perturbations in the early universe. The rate at which these classical black holes nucleate is given by Carr and Hawking [6].

Here, we focus our attention on the cosmological consequences of black holes formed due to a different mechanism; quantum gravitational tunneling from hot flat space. In a seminal paper, Gross, Perry and Yaffe [7] study the rate of black hole nucleation due to this process. They show that the rate of nucleation per unit volume and unit time with $\hbar = c = k_B = G = 1$ is given by,

$$\Gamma(T) = .87T\left[\frac{\mu}{T}\right]^{\theta}\frac{1}{64\pi^3}e^{-1/16\pi T^2}. \tag{6.1.1}$$

where T is the temperature of the radiation, μ is a parameter close to the Planck mass, and θ is a numerical factor which depends on N_s, the number of spin fields accessible to the system:

$$\theta = \frac{1}{45}\Big(212N_2 - \frac{233}{4}N_{3/2} - 13N_1\frac{7}{4}N_{1/2} + N_0\Big). \tag{6.1.2}$$

[1] A version of this paper has been published: G. Hayward and D. Pavón, *Physical Review D* 40 (1989) 1748.

Expression (6.1.1) is confirmed in a recent paper by Kapusta [8], in which he arrives at essentially the same result by heuristic arguments.

Equation (6.1.1) indicates that at temperatures not far below the Planck temperature a copious production of mini black holes is expected. So it is natural to question what impact, if any, these small objects might have on the very early stages of cosmic evolution. The target of this paper is to answer this question.

Before going any further, it is appropriate to sum up the standard model of a radiation dominated universe. The state equations are those for a perfectly radiative fluid;

$$p = \frac{1}{3}\rho, \tag{6.1.3}$$

$$\rho = \frac{\pi^2}{30} N T_{rad}^4. \tag{6.1.4}$$

Furthermore, the spacetime is taken to be homogeneous, isotropic, and, at least in the early universe, spatially flat. Hence, we get the Friedmann–Robertson–Walker (FRW) metric for a spatially flat cosmology,

$$ds^2 = dt^2 - R^2(t)\Big(dr^2 + r^2(d\theta^2 + sin^2\theta d\phi^2)\Big). \tag{6.1.5}$$

The evolution of the scale factor $R(t)$ is dictated by Einstein's equations

$$\left(\frac{dR}{dt}\right)^2 = \frac{8\pi}{3}\rho R^2, \tag{6.1.6}$$

$$\frac{d^2R}{dt^2} = -\frac{4\pi}{3}(\rho + 3p)R. \tag{6.1.7}$$

These equations, supplemented by the state equations (6.1.3) and (6.1.4), can be integrated to give

$$\rho = \frac{3}{32\pi t^2}, \tag{6.1.8}$$

$$R \propto t^{1/2}, \tag{6.1.9}$$

and

$$T_{rad} = \kappa t^{-1/2}, \tag{6.1.10}$$

where

$$\kappa = \left(\sqrt{\frac{45}{N\pi}} \frac{1}{4\pi} \right)^{1/2}. \tag{6.1.11}$$

Now, using equation (6.1.1), we may express the number of black holes per unit comoving volume at time t as

$$n \sim \frac{1}{R(t)^3} \int_{t^*}^{t} R^3(\tau)\Gamma(T(\tau))d\tau. \tag{6.1.12}$$

where t^* is the time of formation of a black hole which would have just evaporated at time t. Further, we express the density of black holes as

$$\rho_{bh} = \frac{1}{R(t)^3} \int_{t^*}^{t} R(\tau)^3 M(t,\tau)\Gamma(T(\tau))d\tau. \tag{6.1.13}$$

where $M(t, \tau)$ is the mass a black hole would have by time t if it formed at time τ. It is worth stressing that when calculating the density of PBH's formed in the early Universe, we do not account for any black holes formed due to the classical process described by Carr and Hawking. It is easy to show that in the very early universe these "classical" PBH's contribute negligibly to the overall PBH density.

The focus of much attention in this paper is to calculate black hole number and energy densities using expressions (6.1.12) and (6.1.13). To do this we must treat the fundamental issue of how PBH mass evolves with time; this is the subject of section 2. We find that much depends on which fundamental theory of nature is presumed to hold after the Planck era. In section 3, we consider specifically three candidate theories; the standard model [SU(3)×SU(2)×U(1)], the supersymmetric standard model, and supersymmetric SU(5). The theories predict a phase, beginning at some time on the order of a Planck time, in which black holes have an energy density comparable to that of ambient radiation. Section 4 treats a fourth theory, SU(5), which predicts a radiation dominated model from the Planck era onward. In section 5, we examine the implications (for instance with respect to baryogenesis and the missing mass problem) of such black hole densities in the very early Universe.

6.2 PBH mass as a function of time

PBH's formed due to quantum instability of hot flat space will be strongly peaked around an initial mass

$$M_{\rm bh}\Big|_{t_{\rm form}} = \frac{1}{8\pi T}\Bigg|_{t_{\rm form}} \tag{6.2.1}$$

where $t_{\rm form}$ is the time of black hole formation and T is the temperature of the ambient radiation. From equation (6.1.10) and the above, the initial mass of PBH's will increase as $t_{\rm form}^{1/2}$.

After the black hole has formed, its interaction with surrounding radiation and with other black holes will determine how its mass changes with time. Let us examine first interactions of black holes with each other.

Note that the relative velocity of neighboring black holes due to Hubble expansion is

$$v_{\rm exp} = \frac{d}{dt}\left(n^{-1/3}\right), \tag{6.2.2}$$

where n is the number density of black holes. Assuming that the total number of black holes in a comoving volume is approximately constant, we have

$$v_{\rm exp} = n^{-1/3}\frac{\dot{R}}{R}. \tag{6.2.3}$$

Meanwhile, the velocity required for a black hole to escape the gravitational pull of its nearest neighbor is

$$v_{\rm esc} = \sqrt{4m\ n^{1/3}}, \tag{6.2.4}$$

where m is the mass of an average black hole. Noting that by energy conservation $\dot{R}/R = \sqrt{8\pi/3(\rho_{\rm rad} + \rho_{\rm bh})}$, and that $\rho_{\rm bh} = nm$, we compare (6.2.3) and (6.2.4) to find that $v_{\rm exp} \geq v_{\rm esc}$ for all possible values of $\rho_{\rm rad}$ and $\rho_{\rm bh}$. Thus, we conclude that black hole/black hole collisions do not occur frequently enough to significantly affect the mass spectrum of black holes in the early universe.

We now examine how any interaction between black holes and surrounding radiation affects the evolution of black hole mass. Even though the black holes form at the same temperature as their surroundings, one might imagine that cooling of the surrounding radiation due to cosmological expansion would cause the black holes to begin evaporating immediately after formation. On the other hand, if the black hole begins absorbing radiation after formation so that its mass increases, evaporation can be forestalled. Indeed, if the black hole mass increases at least as fast as $M_{\rm bh} \propto t^{1/2}$, then it will remain cooler than its surroundings indefinitely and, hence, never evaporate. To determine when (if ever) a typical black hole begins evaporating, we must examine the mean free time of interaction between black holes and surrounding radiation.

The average time of interaction may be expressed as

$$\tau_{\rm int} = \frac{1}{n\sigma}. \tag{6.2.5}$$

where σ is the black hole cross section. Further, we have $\sigma = 4\pi R_{\rm int}^2$ where $R_{\rm int} = 3m$ is the radius of photon capture and m is the average mass of a black hole. Substituting into (6.2.5), and noting that $\rho_{\rm bh} = nm$, we have

$$\tau_{\rm int} = \frac{1}{36\pi m \rho_{\rm bh}}. \tag{6.2.6}$$

This characteristic time between interactions should be compared with the dynamic time associated with Hubble expansion,

$$t_{\text{exp}} = \frac{R}{\dot{R}}. \tag{6.2.7}$$

If $\tau_{\text{int}} \ll t_{\text{exp}}$ then the black hole thermally interacts with surrounding radiation. This thermal system of radiation and black hole is inherently unstable since black holes have negative specific heat. On the other hand, if $\tau_{\text{int}} \geq t_{\text{exp}}$, then the black hole will not interact thermally with surrounding radiation and, hence, it will evaporate freely. We shall find that for all cases of interest to us here $\tau_{\text{int}} \geq t_{\text{exp}}$ and, accordingly, we assume that black holes begin evaporating immediately after forming.

Now, for a freely evaporating black hole, we have by the Stefan-Boltzmann law,

$$\frac{dM}{dt} = \frac{1}{8\pi}\frac{d}{dt}\left(\frac{1}{T}\right) = -\frac{N}{(8\pi)^3 M^2}. \tag{6.2.8}$$

Integration yields,

$$M(t,\tau) = \frac{1}{8\pi}\left[\left[\frac{\tau}{\kappa^2}\right]^{3/2} + 3N(\tau - t)\right]^{1/3}, \tag{6.2.9}$$

where we use equations (6.1.10), (6.1.11), and (6.2.1) to define the mass of the black hole at initial time τ.

6.3 Standard Model, Supersymmetric Standard Model and Supersymmetric SU(5)

We now examine specifically the role black holes play in three different theories: the standard model (SM), supersymmetric (SUSY) SM, and SUSY SU(5). (Since string theories are expected to resemble either SM or SUSY SM at times later than the Planck time, they may be included as well.) It is possible to consider these theories as a group because their values of θ—defined by expression (6.1.3)—are similar and, consequently, they lead to similar black hole densities in the early universe. They predict that flat space is so unstable at the Planck era that black holes quickly make an important contribution to the energy density of the universe.

Let us denote by t_{crit} the time at which ρ_{bh}, calculated using (6.1.13), is approximately half the total energy density, ρ_{tot}, where $\rho_{\text{tot}} = \rho_{\text{rad}} + \rho_{\text{bh}} \simeq \frac{3}{32\pi t^2}$. Further, let $\gamma = (16\pi\kappa^2)^{-1}$ where κ is defined in equation (6.1.11). Then we have from (6.1.1) and (6.1.13) assuming $\mu = 1$ and the radiation dominated model,

$$\rho_{\text{bh}} = \frac{.87\kappa^{(1-\theta)}}{64\pi^3 R(t)^3} I(t), \qquad (6.3.1)$$

where

$$I(t) \equiv \int_{t^*}^{t} R(\tau)^3 \tau^{-0.5(1+\theta)} M(t,\tau) e^{-\gamma\tau} d\tau. \qquad (6.3.2)$$

Then t_{crit} is given implicitly by

$$t_{\text{crit}} = \left[\frac{3\pi^2}{.87 I(t)(16\pi\gamma)^{-0.5(1-\theta)}}\right]^2. \qquad (6.3.3)$$

Table 6.1 lists t_{crit} for the three theories.

To obtain the results of Table 6.1, we assumed that: 1) the density of black holes at $t = 0$ is zero, 2) the probability of black hole formation before $t = 1t_P$ is zero, 3) the black holes begin evaporating freely immediately after formation. Even with these conservative assumptions, we find that the black hole energy density approaches the energy density of the surrounding radiation within about a Planck time (ie. by $\approx 2t_P$).

After ρ_{bh} has become comparable to ρ_{rad} it is reasonable to expect that a steady state would be achieved where

$$\rho_{\text{bh}} \simeq \beta \rho_{\text{rad}} \qquad (6.3.4)$$

Theory	N	θ	t_{crit}
SM	62	3.083	2.5
SUSY SM	132	3.656	1.7
SUSY SU(5)	242	3.000	2.6
SU(5)	104	0.283	

Table 6.1: This table lists for each theory the number, N, of relatively massless fields, an associated parameter θ, and estimates in planck units for t_{crit}, the time at which $\rho_{\text{bh}} \simeq \rho_{\text{rad}}$.

where $\beta \approx$ const. To see this, note that as $\rho_{\text{bh}} \to \rho_{\text{rad}}$ the probability of black hole formation out of radiation will be damped. Meanwhile, a natural lower bound on the ratio $\rho_{\text{bh}}/\rho_{\text{rad}}$ is provided by the high probability of black hole formation in a radiation dominated model and the cosmological redshifting of radiation. We conclude that these three theories all predict that after $t \sim 1t_P$, the Universe enters a phase where black holes and radiation are of comparable energy density in a highly interactive binary mixture. We will refer to this period as the binary phase.

To model the behavior of the universe during the binary phase, we take (6.3.4) to hold and take β to be a constant of order unity. We have

$$\rho = \rho_{\text{bh}} + \rho_{\text{rad}} = (1+\beta)\rho_{\text{rad}}. \tag{6.3.5}$$

Einstein's equations with the usual approximation that the spacetime of the early universe is flat give

$$\frac{dR}{dt} = \left[\frac{8\pi\rho}{3}\right]^{\frac{1}{2}} R, \tag{6.3.6}$$

and

$$d\rho = -3(\rho + p)\frac{dR}{R}, \tag{6.3.7}$$

where the pressure is

$$p = \frac{1}{3}\rho_{\rm rad} = \alpha\rho \tag{6.3.8}$$

and $\alpha = \frac{1}{3(1+\beta)}$ We solve (6.3.6) and (6.3.7) with (6.3.8) to obtain,

$$\rho = \frac{1}{6\pi(1+\alpha)^2 t^2}, \tag{6.3.9}$$

$$R \propto t^{2/3(1+\alpha)}, \tag{6.3.10}$$

and

$$T = \kappa' t^{-1/2}, \tag{6.3.11}$$

where $\kappa' = \left(15\alpha/N\pi^3(1+\alpha)^2\right)^{1/4}$. Note that due to continuous interaction between the black holes and the surrounding radiation, we do not have $\rho_{\rm rad} \propto R^{-4}$. This is because radiation that would otherwise be continuously redshifted spends time in the form of non-relativistic black holes. Equations (6.3.9) and (6.3.10) combine to give that both $\rho_{\rm rad}$ and $\rho_{\rm bh}$ are proportional to $R^{-3(1+\alpha)}$.

To find out how long the binary phase lasts, we must determine how black hole mass varies with time during this phase. As suggested in the previous section, we find that the black holes should begin evaporating immediately after formation. To show this, we examine whether the condition $\tau_{\rm int} \leq t_{\rm exp}$ is satisfied. With equations (6.2.6), (6.3.4), (6.3.5) and (6.3.9) and with

$$m < \frac{M(t,t)}{2} = \frac{t^{1/2}}{16\pi\kappa'}, \tag{6.3.12}$$

we have

$$\tau_{\rm int} > \frac{4\pi}{3\beta}\kappa'(1+\alpha)^2(1+\beta)t^{3/2}. \qquad (6.3.13)$$

Furthermore, from (6.3.10) we have during the binary phase that

$$t_{\rm exp} = \frac{R}{\dot{R}} = \frac{3}{2}(1+\alpha)t. \qquad (6.3.14)$$

Comparing (6.3.13) and (6.3.14) and recalling that $\alpha = \frac{1}{3(1+\beta)}$, we have that $\tau_{\rm int} > t_{\rm exp}$ so long as

$$t > \left[\frac{9}{16}(1-3\alpha)\right]^2\left[\frac{15}{N}\pi\alpha(1+\alpha)^2\right]^{-1/2}. \qquad (6.3.15)$$

Direct substitution into (6.3.15) reveals that $\tau_{\rm int} > t_{\rm exp}$ for all times greater than t_P so long as $\beta \leq 5$. Even when $\beta \gg 1$, the time at which the thermal condition fails increases only as $\beta^{1/2}$. Hence, we conclude that for all mixtures of radiation and black holes likely to arise due to these theories, the thermal condition will have failed either before the binary phase begins or shortly after it begins. We assume, therefore, that black holes begin evaporating freely immediately after formation.

It remains to estimate the time at which the binary phase ends. One estimate for the end time, $t_{\rm end}$, would be the time at which the total mass of black holes within a comoving volume predicted using equation (6.1.13) decreases too quickly to maintain $\rho_{\rm bh} = \beta\rho_{\rm rad}$. The energy density of the black holes near the end of the binary phase will be given by

$$\rho_{\rm bh} \propto \int_{t^*}^{t} M(t,\tau)\tau^{2/(1+\alpha)+0.5(\theta-1)}e^{-\gamma\tau}d\tau. \qquad (6.3.16)$$

where t^* is the time of formation for a black hole which would just evaporate at time t, $\gamma = [16\pi(\kappa')^2]^{-1}$, and κ' is defined beneath equation (6.3.11). At the end of the binary phase, the total mass of black holes within a comoving volume, $M_{\rm bh} = \rho_{\rm bh}R^3$, calculated using (6.3.16), will decrease more rapidly than the total

	$\beta = 0.1$		$\beta = 1$		$\beta = 10$	
Theory	t_{low}	t_{high}	t_{low}	t_{high}	t_{low}	t_{high}
SM	12.6	114	14.4	82	16.7	75
SUSY SM	8.7	64	9.9	44	11.5	38
SUSY SU(5)	5.8	23	6.5	14	7.6	12

Table 6.2: Listing in Planck units of upper and lower estimates for the end time of the binary phase assuming different values for $\beta \equiv \frac{\rho_{bh}}{\rho_{rad}}$.

comoving black hole mass required to maintain $\rho_{\text{bh}} = \beta\rho_{\text{rad}}$. This condition reduces to

$$M(t,t)t^{2/(1+\alpha)+0.5(\theta-1)}e^{-\gamma t} - \frac{N}{(8\pi)^3}\int_{t^*}^{t}\frac{\tau^{2/(1+\alpha)+0.5(\theta-1)}}{M(t,\tau)^2}e^{-\gamma\tau}d\tau \leq -\left[\frac{2\alpha}{6\pi(1+\alpha)^3}\right]t^{-(1+3\alpha)/(1+\alpha)} \quad (6.3.17)$$

The difficulty with an estimate for the end time of the binary phase obtained in this way, is that we actually overcompensate for the effects of evaporation by using the undamped nucleation probability given in equation (6.1.1) to apply over the entire range of integration from t^* to t_{end}. Hence, we list in Table 6.2. the estimates obtained by this method (computed using numerical integration) as lower bounds for the end time.

An upper bound can be found by calculating the time at which ρ_{bh} calculated with equation (6.1.13) becomes smaller than ρ_{bh} calculated using equation (6.3.9). This method actually overestimates the end time because it assumes that black holes form with the undamped probability between t^* and t_{end}. Estimates for the end time obtained using this method are listed in Table 6.2. as upper bounds on t_{end}.

Table 6.2. shows that all three theories we consider in this section predict that the binary phase ends at some time, t_{end}, ranging from approximately ten to a hundred Planck times. The major factor which influences t_{end} is the time dependence of the functions $\Gamma(T)$ and $M(t,\tau)$. Changes to either of these two functions could have a significant effect on the duration of the period in which black holes make a significant contribution to the energy density of the universe.

Finally, it is important to note that there is no sharp transition from binary phase to radiation dominated phase. Even after the total mass of the black holes in a comoving volume begins to decrease, redshifting of radiation will prolong the period over which black holes will contribute significantly to the energy density of the universe. However, exponential damping in the rate of black hole nucleation predicted by (6.1.13), suggests that the black holes will not contribute significantly beyond $t \simeq t_{end} + \frac{1}{\gamma}$.

6.4 SU(5)

In this section, we investigate the role of PBH's in the early universe under SU(5). We find that the black holes do not thermally interact with ambient radiation ($\tau_{int} \gg t_{exp}$) and, hence, they should begin evaporating shortly after forming. We also find that SU(5) predicts a radiation dominated cosmology from the Planck era onward with the PBH energy density exponentially damped for large times.

First, it is worth noting just how the low θ factor of SU(5) reduces the probability of black hole formation. Recall that for the three theories discussed in the previous section, ρ_{bh} becomes comparable to ρ_{rad} within about a Planck time even if we assume the PBH begin evaporating immediately after forming. For SU(5), by contrast, numerical integration reveals that even if the PBH's do not evaporate at all, we do not have $\rho_{\text{bh}} \sim \rho_{\text{rad}}$ until $t \sim 9000 t_P$. While this result is not directly meaningful (since evaporation effects cannot be ignored), it does show that we can safely assume a radiation dominated model for times $t \leq 10^3 t_P$.

We now question how PBH mass evolves with time under the SU(5) model. If $\tau_{\text{int}} >> t_{\text{exp}}$ we would conclude that the PBH begin evaporating immediately after forming. At first glance, however, it would appear that any estimate of τ_{int} will itself depend on an assumption about how PBH mass evolves with time. The key to resolving this apparently self reflexive problem is provided by numerical calculations with different trial functions for $M(t, \tau)$. One finds that regardless of how the PBH's evolve with time, we must have initially $\tau_{\text{int}} \gg t_{\text{exp}}$. Consequently, the only self consistent assumption is that the black holes begin evaporating immediately after formation.

With this, $M(t, \tau)$ is given by equation (6.2.9) and we can calculate ρ_{bh} as a function of time. We find that at no time does ρ_{bh} approach ρ_{rad}; the model remains radiation dominated from the Planck era onward. Figure 6.1 is a graph of $\rho_{\text{bh}}/\rho_{\text{rad}}$ versus time. Note that this ratio achieves a maximum value of .0045 at $t = 7.5 t_P$. After this time the ratio drops off exponentially.

6.5 Implications

Perhaps the most interesting application of our findings is to the problem of baryogenesis. Lindley [9] has observed that the baryon number to photon ratio $n_B/n_\gamma = 10^{-9}$ can be obtained if the universe is assumed to be dominated at $t \sim 100 t_P$ by black holes with $m \sim 100 m_p$, The prime difficulty with Lindley's

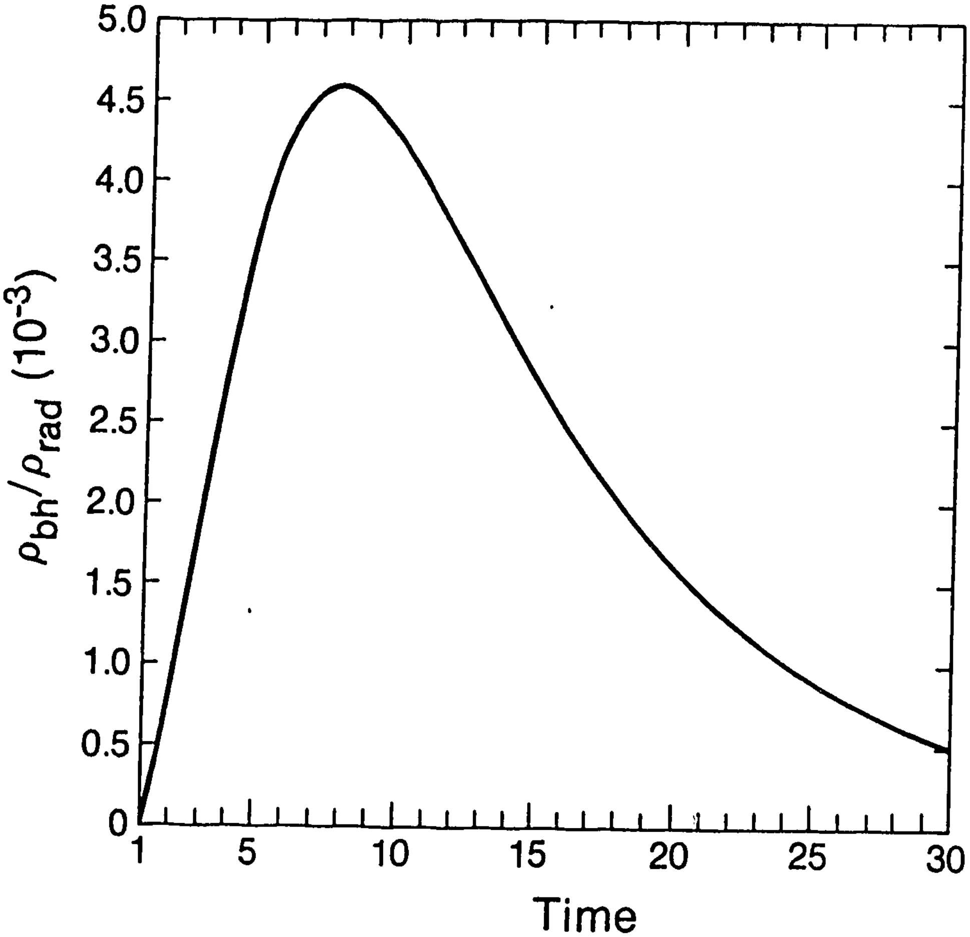

Figure 6.1: Graph of $\frac{\rho_{bh}}{\rho_{rad}}$ as a function of time for SU(5).

proposal, as he himself points out [10], is that his assumption of a black hole dominated cosmology at $t \sim 100t_P$ was totally ***ad hoc.*** It appears on the basis of our findings of section III., however, that three fundamental theories predict a cosmology which may approximate Lindley's hypothetical model.

We conclude that SM, SUSY SM, and SUSY SU(5) might well predict the observed baryon number to photon ratio. The final answer on this score, however, must await a more detailed analysis than we offer here.

It is also worth noting that an inflationary period at the GUT scale would wipe out all trace of any prior $\frac{n_B}{n_\gamma}$ ratio. So if it should result that one or more of the theories we have discussed actually predicts the observed n_B/n_γ, this success might be interpreted as evidence either for a non-inflationary cosmology or for primordial inflation at the Planck scale.

Another point worthy of note is that we have assumed throughout our analysis that black holes evaporate completely. However, it has been argued (eg. Hayward [11] and MacGibbon [4]) that evaporating black holes may actually leave stable Planck mass residues. Indeed, MacGibbon suggests that such relics of PBH's may account for the 'missing mass' in a FRW cosmology. Our analysis casts much doubt on this possibility. All four of the theories we have considered would certainly predict $\rho_{\rm bh} > \rho_{\rm rad}$ for t greater than say $10^4 t_P$ if the black holes left Planck mass residues. In the absence of inflation, this would mean that by today $\rho_{\rm bh}$ would equal $\rho_{\rm tot}$ to extremely high precision. This result is not consistent with the observed density $\rho_{\rm obs} \geq .01\rho_{crit}$.

In conclusion, we have argued that three theories—SM, SUSY SM, and SUSY SU(5)—predict a 'binary phase' lasting between ten and a hundred Planck times in which black holes and radiation are of comparable density. A fourth theory, SU(5), predicts a radiation dominated cosmology from the Planck era onward.

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CHAPTER 7

GENERAL DISCUSSION AND CONCLUSIONS

In[1] this final chapter, I provide the basis for a generalized theory of thermodynamics. This theory applies to a very broad class of thermal systems; in particular, it applies to non-static, non-spherically symmetric systems which include event horizons and/or matter distributions. The general first law derives immediately from the action functional; thermodynamic quantities relate to the boundary's intrinsic 3-metric components and their conjugate momenta. I show how the analysis may be extended to different thermal ensembles—in particular, the microcanonical ensemble—and discuss cases for which there is not a connected boundary to the system. I also present generalized versions of the zeroth, second, and third laws of thermodynamics. All thermodynamic laws relate to basic properties of the Euclidean action and its variations.

7.1 Introduction

In 1973, Bardeen, Carter, and Hawking published a seminal paper entitled "The four laws of black hole dynamics" [1]. They showed that black holes were governed by dynamical laws closely analogous to the laws of classical thermodynamics. When Hawking discovered that black holes emit radiation with a thermal spectrum [2], it became clear that the link between black hole dynamics and classical thermodynamics was more than just analogy. In the years since, much work has been done on "black hole thermodynamics" and, more generally, "horizon thermody-

[1] A version of this Chapter has been submitted to *Physical Review D*.

namics". However, there still persists a widespread belief that the thermodynamic properties of horizons are fundamentally distinct from the thermodynamic properties of classical systems. A general theory of the thermodynamics of systems which include matter and/or horizons is lacking.

In Chapter 3, I derived a general first law for static, spherically symmetric systems which include a matter distribution and either a black hole or a cosmological horizon. This law obtains directly from the Euclidean action for such systems. In contrast to the form of the first law proposed by Bardeen, Carter and Hawking [1] and the spirit of much current research, it makes no distinction between the thermodynamic properties of horizons and matter: both are taken together to constitute a single system with uniquely defined thermodynamic properties.

However, this 'general' first law has limitations. Most importantly, it gives no indication of how one might treat non-static and non-spherically symmetric systems. Also, the calculations I used to derive the law were somewhat involved. Considering the simplicity of the results obtained, one suspects there is some deeper, more general way in which to understand what is going on.

Ideally, one would also like to obtain general formulations of the other laws of thermodynamics. Given the connection between the classical Euclidean action of a system and its free energy, one suspects that the laws of thermodynamics must relate to basic properties of the action.

In Section 7.2, I present a general formulation of the first law of thermodynamics not limited to static or spherically symmetric systems. This law derives immediately from the classical Euclidean action and is the basis for a general theory of thermodynamics. In Section 7.3, I show how to extend the treatment to systems with connected boundaries at which microcanonical boundary constraints are imposed. Section 7.4 extends the treatment to manifolds with non-connected boundaries or with no boundary at all. In Sections 7.5, 7.6, and 7.7, I present generalized versions of the zeroth, second and third laws of thermodynamics respectively. All of these generalized laws relate directly to properties of the Euclidean action and its variations.

It is valuable now to highlight how the connection between thermodynamics and the Euclidean action arises.

The basic quantity from which quantum statistical mechanics derives is the partition function,

$$Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right), \tag{7.1.1}$$

in which β is the inverse temperature and H is the Hamiltonian of the system. [Here and throughout this paper $G = c = k = \hbar = 1$.] It is well known (see for instance, Ref. [3]) that this partition function may be expressed in terms of a Euclidean path integral

$$Z = \int \mathcal{D}\left[g_{\mu\nu}, \phi\right] \mathrm{e}^{-I[g_{\mu\nu},\phi]}. \tag{7.1.2}$$

Here, I is the Euclidean action appropriate to the system and is a functional of the metric functions $g_{\mu\nu}(x)$ and the matter fields (which I formally denote as $\phi(x)$). The path integral is over all metric and matter field configurations which satisfy certain boundary constraints. Some further remarks on the significance of this path integral will be helpful.

First, recognize that the path integral (7.1.2) is also the basic quantity of interest in the Euclidean path integral approach to quantum gravity. In the context of quantum cosmology, this path integral is interpreted as the wave function of the Universe [4,5]. While all the analysis of this paper is performed in the context of gravitational statistical mechanics, it may, with minor revisions, be reset in a quantum cosmological setting.

Second, note that while expression (7.1.1) for the partition function is only well defined for systems in which β is neither a function of position nor time, the path integral (7.1.2) has the potential to apply to a much broader class of systems. For gravitating systems, it is well established that local temperature varies with spatial position due to gravitational redshifting. Further, one would wish to address the dynamics of non-static systems for which the temperature might vary with time. It is therefore natural to consider (7.1.2) as the basic expression for the partition function and note that it reduces to the more familiar expression (7.1.1) in special cases.

Third, recall that, as a partition function, Z is characterized by certain constraints on the system (normally boundary constraints). The choice of constraints determines the statistical ensemble to which the system belongs. Changing the constraint functions causes the system to transfer to a different statistical ensemble in which its mean dynamical properties may be greatly different. Mathematically, the change in the partition function provoked by a change in constraints traces to the fact that the appropriate form for the Euclidean action depends on the constraints. One requires that the action have a well defined variational principle with respect to a given variational class of the field variables. The effects of different choices of boundary constraints on the appropriate form of the gravitational action, and thereby on the partition function, has been addressed by Brown *et al* [6] for static, spherically symmetric vacuum solutions with black hole topology.

Now review how the connection between the partition function and thermodynamics arises. Let

$$J = \ln Z. \tag{7.1.3}$$

In quantum field theory, J is the effective action. In statistical mechanics, J is the Massieu function appropriate to a given ensemble. [The value of using Massieu functions to describe the statistical mechanics of gravitating systems—rather than the more standard free energy formalism—was recognized by Brown *et al.* [6].]

For instance, consider a static, spherically symmetric system for which one chooses to fix the energy E, the surface area, A, and the conserved particle numbers, N_i of the system. These constraints correspond to what are known classically as microcanonical constraints. [Note when a gravitational field is incorporated—even a Newtonian one—the spatial three–symmetry is broken. For static, spherically symmetric problems, the analogue of fixing spatial three–volume is then to fix the boundary surface area.] The Massieu function, associated with these constraints is interpreted as the statistical mechanical entropy,

$$J\,(E, A, N_i) = S\,(E, A, N_i)\,. \tag{7.1.4}$$

The variation of this Massieu function with respect to E, A, and N_i is the 'first law of statistical mechanics' appropriate to the microcanonical ensemble;

$$\delta S = \langle\beta\rangle\,\delta E - \langle p_{\mathrm{A}}\rangle\,\delta A + \sum_i \langle\alpha_i\rangle N_i, \tag{7.1.5}$$

where, for instance, $\langle\beta\rangle \equiv \left(\frac{\partial S}{\partial E}\right)_{A,N_i}$ is the mean statistical inverse temperature.

In the thermodynamic limit (e.g. the system is of a macroscopic scale), the partition function becomes very sharply peaked around the classical solution of minimum action, which I label I_0. Expand around this minimum action to obtain [3,6],

$$J = -I_0 + \text{corrections}. \tag{7.1.6}$$

The thermal (or equivalently, 'stationary phase') approximation ignores the correction terms and defines a thermal Massieu function $J_{\text{thermal}} = -I_0 \approx J$. The first law of thermodynamics (in its microcanonical form) is then,

$$\delta J_{\text{thermal}} = -\delta I_0 = \delta S = \beta\, \delta E - p_{\text{A}}\, \delta A + \sum_i \alpha_i\, \delta N_i. \tag{7.1.7}$$

All quantities in the above expression are now *thermal* approximations to the statistical quantities. Also, one identifies $\lambda = \beta^{-1} p_{\text{A}}$ with a thermal 'surface pressure' and $\mu_i = beta^{-1}\alpha_i$ with the thermal chemical potentials associated with conserved particle numbers N_i.

To go from the thermal Massieu function appropriate to one set of constraints to the thermal Massieu function appropriate to a different set of constraints one employs a Legendre transformation. Thus,

$$\begin{aligned} J_{\text{thermal}}(\beta, A, N_i) &= J_{\text{thermal}}(E, A, N_i) - E\left(\frac{\partial}{\partial E} J_{\text{thermal}}(E, A, N_i)\right)_{A,N_i} \\ &= S - \beta E = -\beta F, \end{aligned} \tag{7.1.8}$$

where F is the Helmholtz free energy. By similar Legendre transformations, the thermal Massieu functions associated with any set of constraints may be determined.

From the above it is clear that the variation of the classical Euclidean action with respect to the constraint data is the first law of thermodynamics. In the next section, I obtain a general expression for this variation. To do this, I employ the Arnowitt–Deser–Misner (ADM) 3 + 1 formalism. It is valuable to review this formalism here.

Consider a general manifold $\mathcal{M}$ with four metric $g_{\mu\nu}$ assumed to be smooth (eg. C^{∞}) throughout the manifold [7]. Suppose, for the moment that the manifold has a connected boundary, $\partial\mathcal{M}$. Choose a $3+1$ nesting of the four geometry such that a *spatial* coordinate y parameterizes the 3–surfaces with y varying from 0 to 1. Without loss of generality, identify the surface Σ_1 at $y = 1$ with the boundary of the manifold. The locus of points Σ_0 at $y = 0$ corresponds to a coordinate singularity of the $3+1$ decomposition (see, for instance [8,9]).

The Euclidean line element in the $3+1$ formalism is then,

$$ds^2 = \left(N^2 + N_i N^i\right) dy^2 + 2N_i\, dy\, dx^i + h_{ij}\, dx^i\, dx^j. \tag{7.1.9}$$

Here N is the lapse function and N^i is the shift vector. Latin indices extend from 0 to 2. The Euclidean time coordinate, τ, is identified with x^0 which, without loss of generality, is taken to range from 0 to 2π.

For the moment, confine attention to the vacuum case. The Euclidean Einstein–Hilbert action associated with the manifold is then

$$I_{\text{E.H.}} = -\frac{1}{16\pi}\int_{\mathcal{M}} R\, g^{1/2}\, d^4x. \tag{7.1.10}$$

Define a Lagrangian scalar density (first order in derivatives with respect to y),

$$\mathcal{L}_{\text{G}} = \frac{N\, h^{1/2}}{16\pi}\left(K_{ij}K^{ij} - K^2 -{}^{(3)}R\right), \tag{7.1.11}$$

where K_{ij} is the extrinsic curvature tensor associated with surfaces of constant y,

$$K_{ij} = \frac{1}{2N}\left(\dot{h}_{ij} -{}^{(3)}\nabla_j N_i -{}^{(3)}\nabla_i N_j\right), \tag{7.1.12}$$

and where $\dot{} \equiv \frac{\partial}{\partial y}$. [Recall that y is a spatial variable so here the overdot does not have its usual meaning of partial differentiation with respect to time.] Obtain,

$$I_{\text{E.H.}} = \int_{\mathcal{M}} \mathcal{L}_{\text{G}}\, d^4x + \frac{1}{8\pi}\int_{\Sigma_1} K\, h^{1/2}\, d^3x - \frac{1}{8\pi}\int_{\Sigma_0} K\, h^{1/2}\, d^3x, \tag{7.1.13}$$

the final term being evaluated in the limit $y \to 0$.

Now define momenta π^{ij} conjugate to h_{ij} by

$$\pi^{ij} \equiv \frac{\partial \mathcal{L}_{\rm G}}{\partial \dot{h}_{ij}} = \frac{1}{16\pi}\left(K^{ij} - h^{ij}K\right) h^{1/2}, \qquad (7.1.14)$$

and, hence (see, for instance, Ref. [8]),

$$I_{\rm E.H.} = -\int_0^1 \left(h_{ij}\dot{\pi}^{ij} + \hat{\mathcal{H}}\right) d^3x\, dy, \qquad (7.1.15)$$

where $\hat{\mathcal{H}} = N_i\mathcal{H}^i + N\mathcal{H}$ and where $N\mathcal{H} = -\frac{1}{8\pi}G^0_0\, g^{1/2}$ and $\mathcal{H}^i = -\frac{1}{8\pi}G^{0i}\, g^{1/2}$.

The extremal conditions in the Hamiltonian representation may actually be obtained by varying the action (7.1.15) with respect to π^{ij}, h_{ij}, N and N^i [10]. Thus,

$$\begin{aligned}\delta I_{\rm E.H.} \;=\; & -\int_0^1 \left\{\left(\dot{\pi}^{ij} + \frac{\partial\hat{\mathcal{H}}}{\partial h_{ij}}\right)\delta h_{ij} + \left(-\dot{h}_{ij} + \frac{\partial\hat{\mathcal{H}}}{\partial \pi^{ij}}\right)\delta\pi^{ij} + \mathcal{H}\,\delta N + \mathcal{H}_i\,\delta N^i\right\} d^3x\, dy \\ & - \int_{\Sigma_1} h_{ij}\delta\pi^{ij} d^3x + \int_{\Sigma_0} h_{ij}\,\delta\pi^{ij} d^3x. \qquad (7.1.16)\end{aligned}$$

It is easy to show that to extremize the action under arbitrary variations, each term in (7.1.16) must vanish *independently*. Hence, for the region $0 < y < 1$, obtain the Einstein equations in the Hamiltonian representation,

$$\begin{aligned}\dot{\pi}^{ij} &= -\frac{\partial\hat{\mathcal{H}}}{\partial h_{ij}} \\ \dot{h}_{ij} &= \frac{\partial\hat{\mathcal{H}}}{\partial \pi^{ij}} \\ \mathcal{H} = 0 & \qquad \mathcal{H}_i = 0. \qquad (7.1.17)\end{aligned}$$

Also, if the variational principle is to be well defined, the variational terms at Σ_0 and Σ_1 must vanish. So, at $y = 0$ and $y = 1$ require either

$$h_{ij} = 0 \quad \text{or} \quad \delta\pi^{ij}. \qquad (7.1.18)$$

Recall that the locus of points at $y = 0$ actually constitutes a coordinate singularity of the $3+1$ metric decomposition. Conditions (7.1.18) should then be understood as smoothness conditions at the coordinate singularity. [For discussions of these smoothness conditions in the Kantowski–Sachs mini–superspace ansatz see Refs. [8,9].]

At Σ_1 the h_{ij} will, in general, not be zero. [If Σ_1 is to be a three–boundary, one requires at least that $\det(h) \neq 0$ there.] Hence, the Einstein–Hilbert action has a well defined variational principle on $\mathcal{M}$ only if the momenta π^{ij} are fixed on the boundary (i.e. $\delta\pi^{ij} = 0$ there).

However, in many standard problems, one is interested in fixing not the π^{ij} but rather the intrinsic three–metric components h_{ij} on the boundary. [In a quantum context, it is, of course, not possible to fix *both* a field variable and its conjugate momentum at the same place and time.] To obtain an action which has a well defined variational principle with h_{ij} fixed on the boundary, subtract the boundary term [11],

$$\int_{\Sigma_1} \pi^{ij} h_{ij}\, d^3x = -\frac{1}{8\pi}\int_{\partial\mathcal{M}} K\sqrt{h}\, d^3x. \tag{7.1.19}$$

Also, it is often useful (although strictly unnecessary) to normalize the action so that a flat spacetime with the same 3–boundary has zero action [3]. The appropriate normalizing factor is

$$\int_{\Sigma_1} \left(\pi^{ij}\right)_0 h_{ij}\, d^3x = \int_{\Sigma_1} K_0\, h^{1/2}\, d^3x \tag{7.1.20}$$

where K_0 is the trace of the extrinsic curvature of the boundary as measured in a flat 4–metric. The 'Gibbons Hawking' action is then

$$\begin{aligned} I_{\text{G.H.}} &= I_{\text{E.H.}} - \frac{1}{8\pi}\int_{\partial\mathcal{M}} [K]\, h^{1/2}\, d^3x \\ &= I_{\text{E.H.}} + \int_{\Sigma_1} \left[\pi^{ij}\right] h_{ij}\, d^3x, \end{aligned} \tag{7.1.21}$$

where square brackets indicate Gibbons–Hawking normalization (eg. $[K] \equiv K - K_0$).

The variation terms at the boundary become

$$\delta I_{\mathrm{G.H.}}\big|_{\Sigma_1} = \int_{\Sigma_1} \left[\pi^{ij}\right] \delta h_{ij}\, d^3x, \tag{7.1.22}$$

which clearly vanish if h_{ij} is a fixed function of x^i on the boundary.

An essential point here is that the appropriate form of the gravitational action depends critically on which constraints are imposed on the system. The form of the action is dictated by the essentially mathematical condition that the action have a well defined variational principle for the chosen type of boundary constraints.

To see more clearly the relation between geometric constraints on a system and thermal constraints, confine attention to the special case of a static, spherically symmetric system. For such a system, the inverse temperature is (see, for example, Refs. [12,13])

$$\beta \equiv \int_0^{2\pi} \sqrt{h_{00}}\, d\tau = 2\pi\sqrt{h_{00}} \tag{7.1.23}$$

while the surface area of the boundary is

$$A = \int_{\Sigma_1} \sqrt{h_{11}h_{22}}\, d^2x = 4\pi\; h_{11}\big|_{\Sigma_1}. \tag{7.1.24}$$

So, for a static, spherically symmetric system, fixing the boundary's intrinsic 3-metric fixes its temperature and surface area. These are boundary constraints appropriate to the canonical ensemble which has a Massieu function

$$J(\beta, A) = -\beta E + S. \tag{7.1.25}$$

7.2 The general first law of thermodynamics

Now examine how the general first law merely expresses the variation of the classical action subject to variation of the boundary data. For the sake of generality, do not assume that the system to be described is either static or spherically symmetric. For definiteness, assume that the system has a connected boundary at which the components of the intrinsic 3–metric are constrained (so the Gibbons–Hawking gravitational action is appropriate). Also, for definiteness, assume that the matter action, depends only on a vector field A_μ and its first derivatives. [The extension to different and more complicated matter actions will be obvious.] Define the matter action in terms of a Lagrangian scalar density $\mathcal{L}_{\rm M}$,

$$I_{\rm matter} = \int_{\mathcal{M}} \mathcal{L}_{\rm M}\left(A_\mu,\ \partial_\nu A_\mu\right) d^4x \tag{7.2.1}$$

Then, the variation of the total action is

$$\begin{aligned} \delta I \ &= \ -\frac{1}{16\pi}\int_0^1 \left(G_{\mu\nu} - 8\pi T_{\mu\nu}\right) \delta g^{\mu\nu}\, g^{1/2}\, d^3x\, dy + \int_{\Sigma_0} h_{ij}\, \delta\pi^{ij}\, d^3x + \int_{\Sigma_1} \left[\pi^{ij}\right] \delta h_{ij}\, d^3x \\ &+ \ \int_0^1 \left\{\frac{\partial \mathcal{L}_{\rm M}}{\partial A_\mu} - \partial_\nu \frac{\partial \mathcal{L}_{\rm M}}{\partial A_{\mu;\nu}}\right\} \delta A_\mu\, d^3x\, dy + \int_{\Sigma_1} \pi^i\, \delta A_i\, d^3x - \int_{\Sigma_0} \pi^i\, \delta A_i\, d^3x, \end{aligned} \tag{7.2.2}$$

where

$$\pi^i = \frac{\partial \mathcal{L}_{\rm M}}{\partial \dot{A}_i}. \tag{7.2.3}$$

Focus now on the variation of the classical, smooth action with respect to variations of the boundary data. Since all metrics in the variational group are classical (i.e. satisfy Einstein's equations and the equations of motion of the matter for $0 < y < 1$) the first and fourth terms in (7.2.2) will be identically zero. Also, the variation terms at Σ_0 will be zero by virtue of the assumption of smoothness [14]. Hence, the variation of the classical action I_0 subject to variation of the boundary data is

$$\delta I_0 = \int_{\Sigma_1} \left[\pi^{ij}\right] \delta h_{ij} d^3x + \int_{\Sigma_1} \pi^i \, \delta A_i \, d^3x \tag{7.2.4}$$

Equation (7.2.4) is a version of the general first law in its integral form. [For fixed boundary data, the right hand side of equation (7.2.4) is zero. However, here we are specifically interested the question of how the classical action varies subject to variation of the boundary data.]

For cases in which local thermodynamic quantities at a small three-patch of the boundary are of interest, a differential form of (7.2.4) is useful. Consider then, an infinitesimal solid angle section, $\Delta\mathcal{M}$ of the manifold. In the y direction, this section extends from the coordinate singularity at Σ_0 to the bounding surface at Σ_1. In the three 'angular' directions, x^i : (τ, θ, ϕ), the section extends from some fixed x^i to $x^i + \delta x^i$. The Gibbons–Hawking action for this section is

$$\begin{aligned} I &= \int_0^1 (\mathcal{L}_{\mathrm{G}} + \mathcal{L}_{\mathrm{M}})\, d^3x\, dy - \int_{\Sigma_1} \pi^{ij} h_{ij}\, d^3x + \int_{\Sigma_1} \left[\pi^{ij}\right] h_{ij}\, d^3x + \int_{\Sigma_0} \pi^{ij} h_{ij}\, d^3x \\ &+ \quad \text{boundary terms at fixed } x^i \\ &- \quad \text{boundary terms at } x^i + \delta x^i. \end{aligned} \tag{7.2.5}$$

Assume sufficient smoothness of the metric and matter fields so the boundary terms at x^i cancel those at $x^i + \delta x^i$. Thus, write the action for $\Delta\mathcal{M}$ as

$$I = \mathcal{I}\, d^3x, \tag{7.2.6}$$

where

$$\mathcal{I} = -\frac{1}{16\pi}\int_0^1 R(g)^{1/2}\, d^3x\, dy - \frac{1}{8\pi}[K]\,(h)^{1/2}\Big|_{\Sigma_1} + \int_0^1 \mathcal{L}_{\mathrm{M}}\, dy. \tag{7.2.7}$$

Also, express the thermal Massieu function of $\Delta\mathcal{M}$ as

$$J_{\text{thermal}} = \mathcal{J}_{\text{thermal}}\, d^3x. \tag{7.2.8}$$

Now take the variation of I, impose smoothness conditions at the coordinate singularity along with the field equations for the metric and matter fields to find

$$\mathcal{J}_{\text{thermal}} = -\mathcal{I}_0 = \left[\pi^{ij}\right] \delta h_{ij}\Big|_{\Sigma_1} + \pi^i \, \delta A_i\Big|_{\Sigma_1} . \tag{7.2.9}$$

This is a 'local first law of thermodynamics'. It represents the variation of a Massieu three-density subject to variations of the constraint data at a small three-patch of the boundary.

a) Global thermodynamics of static, spherically symmetric systems

To see more clearly the thermodynamic significance of equations (7.2.4) and (7.2.9), it is valuable to first confine attention to examples of static, spherically symmetric systems.

Consider, for instance, the case in which the metric is coupled to a gauge field A_μ and the matter action has the form

$$I_{\text{m}} = \frac{1}{16\pi} \int_0^1 F^{\mu\nu} F_{\mu\nu} \, g^{1/2} \, d^3x \, dy, \tag{7.2.10}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. In the static, spherically symmetric case, it is sufficient to consider A_μ of the form

$$A_\mu \, dx^\mu = A_0(y) dx^0. \tag{7.2.11}$$

For this case, solving Einstein's equations yields the Reissner–Nordström solution.

$$ds^2 = h_{00}(y) d\tau^2 + N(y)^2 dy^2 + r(y)^2 \, d\Omega^2, \tag{7.2.12}$$

where

$$\begin{aligned} N^{-2} \dot{r}^2 &= 1 - \frac{2M}{r} + \frac{e^2}{r^2} \\ h_{00} &= (\kappa N)^{-2} \, \dot{r}^2 \end{aligned} \tag{7.2.13}$$

and where M, e, and κ are constant. Physically, the solution corresponds to a charged black hole of mass M, charge e. The locus $r(y = 0) \equiv r_+$ corresponds to the outer black hole horizon while the surface at $r(y = 1) \equiv r_1$ is a bounding shell to the black hole system.

Regularity conditions at the outer horizon constrain the relation between β, ϕ, and r_1 on the one hand, and M, e, and κ on the other. One may use these constraints to re-express the metric solution (7.2.12) entirely in terms of the grand canonical boundary data β, ϕ, and r_1 [15].

Thus, it is possible to show [15] that

$$A_0(1) = \frac{\beta\phi}{2\pi i} = \frac{\beta}{2\pi i} N \dot{r}^{-1}\Big|_{\Sigma_1} \left(\frac{e}{r(0)} - \frac{e}{r(1)} \right), \tag{7.2.14}$$

where $\beta = \int_{\Sigma_1} \sqrt{h_{00}}\, d\tau$ is the inverse temperature and ϕ is the charge potential as measured at the bounding shell. Also,

$$\pi^0(1) = \frac{g^{1/2}}{4\pi h_{00} N^2} \dot{A}_0\Big|_{\Sigma_1} = -\frac{ie}{4\pi}. \tag{7.2.15}$$

Now let

$$I_0 = -J_{\text{thermal}} = \beta F. \tag{7.2.16}$$

Then (7.2.4) yields

$$\begin{aligned} \delta F &= \beta^{-1} \left\{ \frac{1}{\pi} \int_{\Sigma_1} \left[\pi^{00}\right] \sqrt{h_{00}}\, d^3x + \frac{1}{2\pi i} \int_{\Sigma_1} \pi^0 \phi \, d^3x - F \right\} \delta\beta \\ &+ \left\{ \frac{2}{\beta} \int_{\Sigma_1} \left[\pi^{11}\right] d^3x \right\} \delta h_{11} + \left\{ \frac{1}{2\pi i} \int_{\Sigma_1} \pi^0 \, d^3x \right\} \delta\phi. \end{aligned} \tag{7.2.17}$$

Equation (7.2.17) reduces to the canonical first law,

$$\delta F = \beta^{-2} S \, \delta\beta - \lambda \, \delta A - Q \, \delta\phi, \tag{7.2.18}$$

if one makes the identifications

$$\begin{aligned} S &\equiv \beta\left\{\frac{1}{\pi}\int_{\Sigma_1}\left[\pi^{00}\right]\sqrt{h_{00}}\,d^3x + \frac{1}{2\pi i}\int_{\Sigma_1}\pi^0\phi\,d^3x - F\right\} \\ \lambda &\equiv -\frac{1}{2\pi\beta}\int_{\partial\mathcal{M}}\left[\pi^{11}\right]\,d^3x \\ Q &= -\frac{1}{2\pi i}\int_{\Sigma_1}\pi^0\,d^3x. \end{aligned} \tag{7.2.19}$$

Calculate these quantities using (7.2.12) and the expression for the free energy [15]

$$F = \beta^{-1}I_0 = r_1\left(1 - N^{-1}\dot{r}\Big|_{\Sigma_1}\right) - \beta^{-1}\pi r_+^2 - Q\phi. \tag{7.2.20}$$

to obtain,

$$\begin{aligned} S &= \pi r_+^2 \\ \lambda &= -\frac{1}{8\pi r_1}\left\{1 - \frac{\dot{r}}{N}\left[1 + \frac{r\dot{h}_{00}}{2h_{00}}\Big|_{\Sigma_1}\right]\right\} \\ Q &= e, \end{aligned} \tag{7.2.21}$$

which are just the standard equations for the entropy, surface pressure and charge of a Reissner–Nordström black hole in the grand canonical ensemble [15].

To obtain the first law in its more usual 'microcanonical' form, perform a Legendre transformation on $J_{\text{thermal}}(\beta, A, N_i)$. Find that the grand canonical free energy F relates to the mean thermal energy E by

$$F = E - \beta^{-1}S - Q\phi. \tag{7.2.22}$$

From this obtain,

$$E = \frac{1}{\pi}\int_{\partial\mathcal{M}}\left[\pi^{00}\right]\sqrt{h_{00}}\,d^3x, \tag{7.2.23}$$

and

$$\delta E = \beta^{-1}\,\delta S - \lambda\,\delta A + \phi\,\delta Q. \tag{7.2.24}$$

Explicit calculation of the quantity E reveals that it agrees with the standard expression for the mean thermal energy of the black hole system as measured at its boundary [15],

$$E = r_1 \left(1 - \left[1 - \frac{r_+}{r_1} \right]^{1/2} \left[1 - \frac{e^2}{r_1 r_+} \right]^{1/2} \right). \tag{7.2.25}$$

As a second example, consider a generic, static, spherically symmetric system which includes a matter distribution and possibly a black hole horizon. [One might equally consider a static, spherically symmetric system which extends from 3–boundary out to a cosmological horizon. Apart from a change of sign in the mean thermal energy and surface pressure [13,16], the results are essentially the same as for the case considered here.]

The action for a generic matter distribution, has the form [12],

$$I_{\text{matter}} = -\int_0^1 p\, g^{1/2}\, d^3x\, dy = \int_0^1 \left(\rho - T\sigma - \sum_i \mu_i n_i \right) g^{1/2}\, d^3x\, dy, \tag{7.2.26}$$

where $p(y)$ is the local pressure of the material and ρ, σ, and n_i are respectively the local energy, entropy, and conserved particle number densities per unit spatial volume. Also, the μ_i are chemical potentials associated with conserved particle number densities n_i. In keeping with the principle of equivalence [12], take

$$\mu_i = \beta^{-1}(y)\alpha_i, \tag{7.2.27}$$

where the α_i are constant (i.e. independent of x^i, y) thermal potentials for the matter.

The classical metric associated with such a matter distribution has the form of (7.2.12) with

$$N^{-2}\dot{r}^2 = 1 - \frac{2m(r)}{r} \tag{7.2.28}$$

and

$$h_{00}(r) = \left(\frac{\beta}{2\pi}\right)^2 \frac{1 - \frac{2m(r)}{r}}{1 - \frac{2m(r_1)}{r_1}} e^{2(\psi(r) - \psi(r_1))}, \tag{7.2.29}$$

where β is the temperature of the boundary and m and ψ satisfy

$$\begin{aligned} m(r) &= \frac{r_+}{2} + 4\pi \int_{r_+}^{r} \rho r^2 \, dr \\ \frac{\partial \psi}{\partial r} &= \frac{4\pi (\rho + p) r}{1 - \frac{2m}{r}}. \end{aligned} \tag{7.2.30}$$

A straightforward calculation [12,13] yields for the classical total action

$$I_0 = \beta r_1 \left(1 - \sqrt{1 - \frac{2m(r_1)}{r_B}}\right) - \pi r_+^2 - \int \sigma \, d^{(3)}V - \sum_i \left\{ \alpha_i \int n_i \, d^{(3)}V \right\}. \tag{7.2.31}$$

where $d^{(3)}V \equiv \sqrt{^{(3)}g} \, d^2x \, dy$ and the last two term are integrated over the spatial Euclidean 3-volume of the manifold.

Note that the action is a function of the constant thermal potentials α_i. The variation of the classical smooth action (obtained in the same way as equation (7.2.4)) is just

$$\delta I = \int_{\Sigma_1} \left[\pi^{ij}\right] \delta h_{ij} \, d^3x - \sum_i \left[\int n_i \, d^{(3)}V\right] \delta \alpha_i. \tag{7.2.32}$$

Analysis similar to that performed above yields

$$\begin{aligned} \delta F &= \beta^{-1} \left\{ \int_0^1 \frac{\left[\pi^{00}\right] \sqrt{h_{00}}}{\pi} \, d^3x - \sum_i \mu_i \int n_i \, d^{(3)}V - F \right\} \delta\beta \\ &+ 2\beta^{-1} \int_{\Sigma_1} \left[\pi^{11}\right] d^3x \, \delta h_{11} - \sum_i \left[\int n_i \, d^{(3)}V\right] \delta \mu_i, \end{aligned} \tag{7.2.33}$$

where $\mu_i = \beta^{-1} \alpha_i$. Recall that for a spherically symmetric system

$$\delta F = \beta^{-2} S \, \delta\beta - \lambda \, \delta A - \sum_i N_i \delta \mu_i. \tag{7.2.34}$$

Using $I_0 = -J_{\text{thermal}}(\beta, A, N_i) = \beta F$ and equation (7.2.31), one obtains,

$$\begin{aligned} S &= \beta\left\{\int_0^1 \frac{[\pi^{00}]\sqrt{h_{00}}}{\pi}\, d^3x - \sum_i \mu_i \int n_i\, d^{(3)}V - F\right\} \\ &= \pi r_+^2 + \int \sigma\, d^{(3)}V \\ &= S_{\text{bh}} + S_{\text{matter}} \end{aligned} \tag{7.2.35}$$

and

$$N_i = \int n_i\, d^{(3)}V \tag{7.2.36}$$

as well as the equation for λ given in (7.2.21).

To transform the canonical first law (7.2.33) to its more usual microcanonical form, perform a Legendre transformation on $J_{\text{thermal}}(\beta, A, N_i)$. One finds that the mean thermal energy and the free energy relate by

$$F = E - \beta^{-1}S - \sum_i \mu_i N_i. \tag{7.2.37}$$

Substitute this into (7.2.35) and (7.2.33 to obtain,

$$E = \int_{\Sigma_1} \frac{[\pi^{00}]\sqrt{h_{00}}}{\pi}\, d^3x \tag{7.2.38}$$

and

$$\delta E = \beta^{-1}\,\delta S - \lambda\,\delta A + \sum_i \mu_i\,\delta N_i. \tag{7.2.39}$$

This is just the first law that was derived at some length in Chapter 3.

Note that in equation (7.2.39), β, μ_i, and λ are derived quantities obtained by taking the partial derivatives of (7.2.38) with respect to S, N_i, and A. The β, μ_i, and λ obtained in this way are precisely the locally redshifted quantities that would be measured at the boundary when the presence of the matter distribution is taken into account [16].

Having shown that equation (7.2.4) reduces to the first law in the static spherically symmetric case, it remains to consider the more general case in which the metric is neither static nor spherically symmetric.

b) 'Local' thermodynamics of bounded systems

Strictly speaking, the classical thermal properties of non-static systems are ill defined. For instance, relation (7.1.23) between the inverse temperature β of a system and the proper period of the Euclidean time variable does not hold for general non-static systems. Standard methods for deriving this relation (see, for instance, [17]) explicitly assume the Hamiltonian of the system to be time independent.

To ascribe thermal properties to non-static systems, require as a necessary condition that

$$t_{\text{dynamic}} >> \delta t_{\text{meas.}}, \tag{7.2.40}$$

where t_{dynamic} is the dynamic time of thermal evolution of the system and $\delta t_{\text{meas.}}$ is the time required to perform *any individual measurement of a given thermal property of the system.* For example, it is sensible to speak of the temperature of a system as a function of time only if the system is approximately static over the time interval required to make a given measurement of the temperature. In principle, $\delta t_{\text{meas.}}$ can be made arbitrarily small, so condition (7.2.40) can be satisfied for any dynamic system. However, as $\delta t_{\text{meas.}} \to 0$, one eventually acquires unacceptable uncertainties in the energy of the system (by virtue of the uncertainty principle).

A more stringent requirement one might make of a non-static thermal system is that

$$\delta t_{\text{meas.}} >> \hbar\beta_l = \hbar/k_{\text{B}}T_l, \tag{7.2.41}$$

where $\beta_l \equiv 1/k_B T_l$ is the 'local' inverse temperature ascribed to the system at the time of measurement. In other words, one requires that over the time interval of measurement, the system appear approximately periodic in Euclidean time with the time interval of measurement corresponding to several 'periods' of Euclidean time.

Taken together, conditions (7.2.40) and (7.2.41) place reasonable limits on the consistency of applying thermal concepts to dynamic systems. For instance, condition (7.2.41) implies that it is only meaningful to ascribe a temperature of $100K$ to a system if one measures that temperature over a time interval greater than 10^{-13} seconds. Condition (7.2.40) further requires that the time scale over which the thermal properties of the system evolve cannot be less than 10^{-13} seconds.

Condition (7.2.41) and similar conditions on δx^1 and δx^2 effectively limit the applicability of thermal concepts to patches of the boundary which are sufficiently large that it is sensible to identify thermal properties for the patch and yet small enough that these thermal properties are sufficiently constant over the entire patch.

An added twist which appears in the treatment of non-static systems is that metrics which are real in the Lorentzian sector are not necessarily real in the Euclidean sector. While equations (7.2.4) and (7.2.9) apply as much to complex metrics as to real ones, in order to avoid issues of interpretation that need not be raised here, limit attention to metrics which have real components in the Euclidean sector.

A further complication which I wish to avoid arises if either h_{01} or h_{02} is non-zero on the boundary. An example of a case in which it would be natural to fix h_{01} to be some non-zero function on the boundary occurs for rotating black hole systems. The action for such systems has been calculated in an intriguing paper by Brown, Martinez, and York [18]. While it would appear possible to extend the analysis of Brown, Martinez, and York to obtain a local version of the first law for systems in which h_{01} and h_{02} are non-zero on the boundary, this would require introducing a $3+1$ split different from the one I have employed here. For simplicity, then confine attention to cases in which $h_{01} = h_{02} = 0$ on the boundary.

Subject to the above constraints, define a 'local inverse temperature', β_l at Lorentzian time t_0 by,

$$\beta_l = 2\pi\sqrt{h_{00}}\Big|_{t_0} . \tag{7.2.42}$$

where $h_{00}^{1/2}\big|_{t_0}$ is the lapse function in the Euclidean sector evaluated at $\tau_0 = it_0$. The rationale for referring to β_l as a 'local inverse temperature' is as follows. So long as condition (7.2.40) is satisfied, $h_{00}(\tau, x^1, x^2, y) \approx h_{00}(\tau_0, x^1, x^2, y)$ over the interval of measurement. Further, by condition (7.2.41), it is possible to identify an approximate local periodicity in Euclidean time,

$$\beta_l = \int_0^{2\pi} \sqrt{h_{00}}\Big|_{\tau_0} d\tau = 2\pi \sqrt{h_{00}}\Big|_{\tau_0} . \tag{7.2.43}$$

In essence, the local temperature over the interval of measurement from t_0 to $t_0 + \delta t_{\text{meas.}}$ agrees with the temperature that would be measured if the system were globally static with $h_{00} = h_{00}|_{t_0}$.

Now consider the thermal Massieu density, $\mathcal{J}_{\text{thermal}} = -\mathcal{I}_0$ given in equation (7.2.9). Let $\mathcal{J}_{\text{thermal}} = -\beta_l\mathcal{F}$ where $\mathcal{F}$ is a local 'free energy scalar density' (i.e. per unit coordinate area and time) as measured at some point on the bounding 3-surface. For definiteness, assume a matter action of the form (7.2.10). Analysis similar to that performed above, yields

$$\delta\mathcal{F} \;=\; \beta_l^{-1}\left\{\frac{[\pi^{00}]\sqrt{h_{00}}}{\pi} + \frac{1}{2\pi i}\pi^0\phi - \mathcal{F}\right\}\delta\beta_l +$$

$$+\ \beta_l^{-1}\left[\pi^{AB}\right]\delta h_{AB}+\frac{1}{2\pi i}\pi^0\,\delta\phi+\beta_l^{-1}\pi^B\,\delta A_B. \qquad (7.2.44)$$

where indices A, B range from 1 to 2 and where, by virtue of the scaling properties of A_0 and Gauss' law, $A_0=\frac{\beta_l\phi}{2\pi i}$.

In this equation, the boundary data β_l, h_{AB}, ϕ and A_B are any functions of x^i which satisfy general thermality conditions of the form (7.2.40) and (7.2.41). In other words, equation (7.2.44) applies to cases in which the boundary data varies with time and from one part of the boundary's spatial cross section to another.

In analogy with the thermodynamics of static systems, define local thermal properties at the boundary by

$$\delta\mathcal{F}=\beta_l^{-2}\mathcal{S}\,\delta\beta-\mathcal{P}^{AB}\,\delta h_{AB}-\mathcal{Q}\,\delta\phi+\mathcal{M}^B\,\delta A_B. \qquad (7.2.45)$$

For instance, a 'local entropy scalar density' at the boundary is

$$\mathcal{S}\equiv\beta_l^2\left(\frac{\partial\mathcal{F}}{\partial\beta_l}\right)_{h_{AB}}=\beta_l\left\{\frac{\left[\pi^{00}\right]\sqrt{h_{00}}}{\pi}+\frac{1}{2\pi i}\pi^0\phi-\mathcal{F}\right\}. \qquad (7.2.46)$$

Local thermal 'pressure scalar densities' $\mathcal{P}^{AB}$ are given by,

$$\mathcal{P}^{AB}=\beta_l^{-1}\left[\pi^{AB}\right], \qquad (7.2.47)$$

and other local thermal properties are obtained similarly by comparing (7.2.44) and (7.2.45). Also, let $\mathcal{F}=\mathcal{E}-\beta_l^{-1}\mathcal{S}-\mathcal{Q}\phi$ to obtain the 'local energy scalar density',

$$\mathcal{E}=\frac{\left[\pi^{00}\right]\sqrt{h_{00}}}{\pi}, \qquad (7.2.48)$$

and the 'local microcanonical first law',

$$\delta\mathcal{E}=\beta_l^{-1}\,\delta\mathcal{S}+\mathcal{P}^{AB}\,\delta h_{AB}+\phi\,\delta\mathcal{Q}+\mathcal{M}^B\,\delta A_B. \qquad (7.2.49)$$

To interpret the physical significance of the local thermal properties defined above, first, note that for the static, spherically symmetric case,

$$\begin{aligned}\int_{\Sigma_1} \mathcal{S}\, d^3x &= S\\ \int_{\Sigma_1} \mathcal{E}\, d^3x &= E\\ \int_{\Sigma_1} \mathcal{Q}\, d^3x &= Q,\end{aligned} \tag{7.2.50}$$

where S, E, and Q are respectively the entropy, entropy and charge of a static, spherically symmetric system given in equations (7.2.19), (7.2.21), and (7.2.23).

For systems which are neither static nor spherically symmetric, a simple interpretation of the local thermal properties derived above is still possible. Let ${}^{(2)}h$ be the determinant of the boundary's intrinsic spatial 2–metric. Then, subject to the thermal constraints (7.2.40) and (7.2.41), the mean thermal energy per unit spatial area of the boundary as measured at x^A and time $x^0 = \tau$ is

$$\varepsilon = \frac{2\pi}{\sqrt{{}^{(2)}h}}\mathcal{E}\left(x^i\right). \tag{7.2.51}$$

Similarly the entropy per unit spatial area at x^A and time τ is

$$s = \frac{2\pi}{\sqrt{{}^{(2)}h}}\mathcal{S}\left(x^i\right). \tag{7.2.52}$$

Also, by virtue of Gauss' law, $\mathcal{Q} = \frac{1}{2\pi}\vec{E}\cdot\vec{n}\sqrt{{}^{(2)}h}$ where $\vec{E}$ is the electric field vector and $\vec{n}$ is the unit normal to the surface. Hence, the electric flux through a spatial 2-patch of the boundary of unit area at time τ is

$$\Phi_{\mathrm{E}} = \frac{2\pi}{\sqrt{{}^{(2)}h}}\mathcal{Q}\left(x^i\right). \tag{7.2.53}$$

While the precise interpretation of the $\mathcal{M}^A$ need not concern us here, these quantities relate to magnetic fields tangential to the spatial 2–boundary of the system and are expected to give information about electric currents in the system by virtue of Ampere's law.

At this point two remarks are in order. First, it is important to note that, formally, the first law relation (7.2.49) applies even to systems which do not satisfy 'thermality' conditions such as (7.2.40) and (7.2.41) and to systems whose metric components are not real on the boundary. Equation (7.2.49) derives directly from (7.2.9) which expresses the variation of the classical action subject to variations of *completely arbitrary* canonical boundary data. In particular, the variational equations (7.2.9) and (7.2.49) are valid even in physical situations which have no 'thermal' interpretation. Ultimately, the validity of equations (7.2.9) and (7.2.49) is constrained only by quantum gravitational effects.

Second, note that *the thermal conjugate of a variable is also its quantum gravitational conjugate.* [Brown *et al.* [6] have pointed this out for static, spherically symmetric systems.] For, instance, the local (un-normalized) energy density, $\mathcal{E}_{\rm B} = \frac{1}{\pi}\pi^{00}\sqrt{h_{00}}$, and the local inverse temperature, $\beta_l = 2\pi\sqrt{h_{00}}$ are thermally conjugate variables (eg. one fixes either one of them but not both at the boundary). They are also quantum gravitationally conjugate variables as can be seen by expressing the York gravitational action as

$$I_{\rm Y} = \int_0^1 \left(\mathcal{E}_{\rm B}\dot{\beta}_l + 2\pi^{0A}\dot{h}_{0A} + \pi^{AB}\dot{h}_{AB} - N\mathcal{H} - N_i\mathcal{H}^i\right), \qquad (7.2.54)$$

where $\mathcal{H}$ and $\mathcal{H}^i$ are functions of β_l, $\mathcal{E}_{\rm B}$, π^{AB}, and h_{AB}.

7.3 Systems at fixed energy

In the above section, I assumed 'canonical boundary conditions' for the gravitational action. In other words, I assumed that the components of the boundary's intrinsic 3-metric, h_{ij}, were to be constrained. In this section, I derive the gravitational action appropriate to 'microcanonical boundary conditions'. Such boundary conditions are appropriate to isolated systems and, so, are of fundamental thermodynamic significance.

For a microcanonical system, it is the energy rather than the temperature which is constrained on the boundary. Ignoring the Gibbons–Hawking normalization constant, the (bare) energy scalar density on the boundary is,

$$\mathcal{E}_{\mathrm{B}} = \frac{1}{\pi}\pi^{00}\sqrt{h_{00}}. \tag{7.3.1}$$

We require a form of the gravitational action appropriate to fixing $\mathcal{E}_{\mathrm{B}}$ on the boundary.

To this end, consider a 'microcanonical, gravitational action' $I_{\mathrm{M.G.}}$ defined by[2]

$$I_{\mathrm{M.G.}} \equiv -\frac{1}{16\pi}\int_0^1 R\, g^{1/2}\, d^3x\, dy + \int_{\Sigma_1} \pi^{ij} h_{ij} - 2\int_{\Sigma_1} \pi^{00}\, h_{00}\, d^3x, \tag{7.3.2}$$

Further, let an action scalar density, $\mathcal{I}_{\mathrm{M.G.}}$ be given by

$$I_{\mathrm{M.G.}} = \int \mathcal{I}_{\mathrm{M.G.}}\, d^3x. \tag{7.3.3}$$

Vary $\mathcal{I}_{\mathrm{M.G.}}$ and integrate by parts to find that the variations at the boundary are

$$\begin{aligned} \delta\mathcal{I}_{\mathrm{M.G.}}|_{\Sigma_1} &= \left\{\pi^{AB}\,\delta h_{AB} - \pi^{00}\,\delta h_{00} - 2h_{00}\,\delta\pi^{00}\right\}\Big|_{\Sigma_1} \\ &= \pi^{AB}\,\delta h_{AB} - \beta_l\,\delta\mathcal{E}_{\mathrm{B}}, \end{aligned} \tag{7.3.4}$$

where the indices A, B range from 1 to 2 and $\beta_l = 2\pi\sqrt{h_{00}}$. Clearly, these are the variations appropriate to fixing h_{AB} and $\mathcal{E}_{\mathrm{B}}$ on the boundary.

[2]After completion of this paper, it has come to my attention that Brown *et al.* perform an integral transform on the canonical partition function to obtain a microcanonical action for vacuum static, spherically symmetric systems [6]. For such systems, the microcanonical action derived below agrees with that derived by Brown *et al.*.

I have called $I_{\text{M.G.}}$ a 'microcanonical' gravitational action. However, whether or not the full action is 'microcanonical' depends on the form of the matter action. One needs to choose a form of the matter action that has a well defined variational principle when the conserved particle numbers are held fixed at the boundary. For instance, if the canonical matter action is given by (7.2.10) the 'microcanonical matter action' is

$$I_{\text{M.M.}} = \frac{1}{16\pi}\int_0^1 F_{\mu\nu}F^{\mu\nu}\, g^{1/2}\, d^3x\, dy - \int_{\Sigma_1} \pi^0 A_0\, d^3x. \qquad (7.3.5)$$

To interpret the thermodynamic significance of $\mathcal{I}_{\text{M}} = \mathcal{I}_{\text{M.G.}} + \mathcal{I}_{\text{M.M.}}$, note (after a tedious but straight forward calculation) that it relates to the Gibbons Hawking normalized canonical 'action density', $\mathcal{I}_0$, by

$$\mathcal{I}_{\text{M}} = \mathcal{I}_0 - \beta_l\mathcal{E} + \beta_l\mathcal{Q}\phi, \qquad (7.3.6)$$

where $\mathcal{E} = [\pi^{00}]\sqrt{h_{00}}$ is the Gibbons-Hawking normalized energy density. But, $\mathcal{I}_0 = \beta_l\mathcal{E} - \mathcal{S} - \beta_l\mathcal{Q}\phi$, so,

$$\mathcal{I}_{\text{M}} = -\mathcal{S}. \qquad (7.3.7)$$

This is the anticipated relation between the microcanonical action and the entropy. [Recall that the weighting factor of the path integral is e^{-I} and that of the microcanonical ensemble is e^{S}.]

Note that the microcanonical gravitational action defined in equation (7.3.2) does not require any normalization factor. The microcanonical action of flat spacetime is zero. This is a very attractive feature since there are strict limitations on the class of spacetimes to which Gibbons-Hawking normalization can be applied [19].

Also note, that varying the classical, smooth microcanonical action with respect to boundary data yields immediately the microcanonical first law (7.2.49).

7.4 Manifolds without a connected boundary

All the analysis of Sections 7.2 and 7.3 assumes a connected boundary to the manifold. However, to have a completely general formulation of thermodynamics, one must consider manifolds with boundaries which are not connected and manifolds without boundary at all.

It is straightforward to extend the analysis of Sections 7.2 and 7.3 to cases in which the manifold has two connected bounding surfaces. Assume, for instance, canonical boundary conditions at both boundaries. Express the metric in the $3+1$ form (7.1.9) with y ranging from 0 to 1. Identify one boundary with the surface $y = 0$ and the other boundary with the surface $y = 1$. The variation of the classical action density is then

$$\delta\mathcal{I}_0 = \left[\pi^{ij}\right] \delta h_{ij}\Big|_{\Sigma_1} - \left[\pi^{ij}\right] \delta h_{ij}\Big|_{\Sigma_0} . \tag{7.4.1}$$

This may then be interpreted as the generalized first law for the system.

For a more familiar form, let $\mathcal{I}_0 = \beta_{l_1}\mathcal{F}_1 - \beta_{l_0}\mathcal{F}_0$ where $\beta_{l_1} = 2\pi\sqrt{h_{00}}\Big|_{\Sigma_1}$ and β_{l_0} is defined similarly at Σ_0. Substitute into (7.4.1) to get

$$\beta_l\, \delta\mathcal{E}\,\Big|_0^1 = \left\{\delta\mathcal{S} + \left[\pi^{AB}\right] \delta h_{AB}\right\}\Big|_0^1 , \tag{7.4.2}$$

where $\mathcal{E}$ and $\mathcal{S}$ are as given in equations (7.2.48) and (7.2.46). In most practical experiments, one would vary conditions at one of the boundaries and keep the data fixed at the other boundary. Under these conditions, equation (7.4.2) only has contributions from the boundary where the variations are being made.

When the system has three or more connected bounding surfaces, the $3+1$ decomposition may still be used. However, coordinate singularities should arise in such cases as they did in the case of a single connected boundary. Since, only the variations of the classical smooth action are of interest, variations along the loci of the coordinate singularities are zero. Hence, one obtains a generalized first law similar to (7.4.2) with variation terms on the right hand side for each of the bounding surfaces.

For compact manifolds without boundary (eg. those considered in Ref. [13]), one expects the first law to relate variations in the classical action to variations in global constraints on the system. For instance, one might consider ensembles in which either the 4–volume or the cosmological constant is constrained. I will treat such ensembles in detail in a separate publication.

As a final note to this discussion, remark that any device used to measure the thermodynamic properties of a manifold without boundary, can itself be viewed as a boundary to the system. Thus, one can define a first law associated with variations of the boundary data *on the measuring device*. In fact, the thermodynamic properties we associate with a system are determined by virtue of the variations at the surface of the measuring device. What one actually measures is variations in the classical action as the measuring device comes into equilibrium with the surrounding manifold.

7.5 The zeroth law of thermodynamics

The classical zeroth law stipulates that two isolated systems brought into thermal contact come to equilibrium at a common temperature. To derive the analogous result in the context of generalized thermodynamics, we must consider microcanonical systems which have a jump discontinuity in $\beta_l = 2\pi\sqrt{h_{00}}$ across some surface.

Address first the broader issue of how jump discontinuities contribute to different forms of the gravitational action; in particular, the York and the Einstein–Hilbert forms. In all cases, assume that the fundamental field variables of the action are continuous and that the jump discontinuity occurs in the conjugate momenta. [Indeed, it is by virtue of continuity in the fundamental field variables that one can identify points across the jump discontinuity at all.] Also, for simplicity, assume that the systems in question have connected boundaries at $y = 0$ and at $y = 1$.

Review the role of jump discontinuities in the York action. This action is of canonical form if the h_{ij} are taken as fundamental field variables. Consider then the contribution to the action of a jump discontinuity in π^{ij} at a surface $y = \alpha$ at which, by hypothesis, h_{ij} is continuous. The York action is

$$\begin{aligned} I_{\mathrm{Y}} &= I_{\mathrm{E.H.}} + \int_{\Sigma_1} \pi^{ij} h_{ij}\, d^3x - \int_{\Sigma_0} \pi^{ij} h_{ij}\, d^3x \\ &= \int_0^1 \left(\pi^{ij}\dot{h}_{ij} - N\mathcal{H} - N_i\mathcal{H}^i\right) d^3x\, dy - \lim_{\varepsilon\to 0}\left\{\int_{\alpha-\varepsilon}^{\alpha+\varepsilon} \frac{\partial}{\partial y}\left(\pi^{ij}h_{ij}\right) d^3x\, dy\right\} \end{aligned} \quad (7.5.1)$$

In the Hamiltonian formulation, $\mathcal{H}$ and $\mathcal{H}^i$ are functions of h_{ij} and π^{ij}. Hence, all terms in the first integrand in (7.5.1) have at most jump discontinuities at $y = \alpha$ and the first term in (7.5.1) does not contribute in the limit $\varepsilon \to 0$. The contribution to the action of the jump discontinuity in π^{ij} is then given entirely by the second integral in (7.5.1),

$$I_{\text{jump}} = -\int_{r=\alpha} \left(\pi^{ij}\Big|_+ - \pi^{ij}\Big|_-\right) h_{ij}\, d^3x. \quad (7.5.2)$$

This is the standard result. In Ref. [8] it is noted that extremizing the action over metrics with jump discontinuities in π^{ij} yields

$$\pi^{ij}\Big|_+ = \pi^{ij}\Big|_-, \quad (7.5.3)$$

that is, smoothness in π^{ij} as part of the 'generalized Einstein equations'. If one includes a matter shell at $y = \alpha$ and extremizes the total action, one obtains the ord aary Einstein equations in the regular part of the manifold and the Israel surface equations at $y = \alpha$ [8].

Now treat the case of the Einstein–Hilbert action. This action has canonical form if one takes the π^{ij} to be fundamental field variables. Focus then on the case in which a jump discontinuity occurs in the h_{ij} at a surface where the π^{ij} are continuous. The action is

$$I_{\text{E.H.}} = -\int_0^1 \left(h_{ij}\dot{\pi}^{ij} + N\mathcal{H} + N_i\mathcal{H}^i \right) d^3x\, dy. \tag{7.5.4}$$

Note by inspection that the jump discontinuity makes no contribution to the action since no term in (7.5.4) has more than a jump discontinuity at $y = \alpha$. Varying the action with respect to this class of metrics yields the variational equation

$$\begin{aligned} \delta I &= -\frac{1}{16\pi}\int_0^{\alpha-} \left(G_{\mu\nu} - 8\pi T_{\mu\nu}\right) g^{1/2}\,\delta g^{\mu\nu}\, d^3x\, dy - \int_{y=\alpha} \left(h_{ij}|_+ - h_{ij}|_- \right) \delta\pi^{ij}\, d^3x \\ &- \frac{1}{16\pi}\int_{\alpha_+}^1 \left(G_{\mu\nu} - 8\pi T_{\mu\nu}\right) g^{1/2}\,\delta g^{\mu\nu}\, d^3x\, dy \end{aligned} \tag{7.5.5}$$

and

$$h_{ij}|_+ = h_{ij}|_- \tag{7.5.6}$$

as part of the generalized Einstein equations.

With the benefit of the above analysis, now consider an experiment in which two initially isolated systems at different temperatures are brought into thermal contact. For simplicity, imagine that an adiabatic wall between two systems has been replaced by a diathermal one.

Since each system is initially isolated (eg. surrounded by an adiabatic wall), the initial energy of each system is constrained. The appropriate action to describe systems of fixed energy, is the microcanonical action derived in Section 7.3,

$$I_{\mathrm{M}} = I_{\mathrm{Y}} - 2\int_{\partial\mathcal{M}} \pi^{00}\, h_{00}\, d^3x + I_{\mathrm{matter}}, \tag{7.5.7}$$

where I_{Y} is the York action. The fundamental field variables for this theory are the h_{AB} and the bare energy scalar density $\mathcal{E}_{\mathrm{B}} = \frac{1}{\pi}\pi^{00}\sqrt{h_{00}}$. The momentum conjugate to $\mathcal{E}_{\mathrm{B}}$ is β_l.

Now replace the adiabatic wall by a diathermal wall. Treat the composite system as a single manifold and take the diathermal wall to be massless and stressless. Choose a 3 + 1 decomposition of the 4–metric such that the shared boundary is the surface $y = \alpha$. The π^{AB} must be continuous across $y = \alpha$ by virtue of the Israel surface equations and the fact that the diathermal wall is stressless. Also, the local un-normalized energy density, $\mathcal{E}_{\mathrm{B}}$, must be continuous across the surface, since the diathermal wall is massless. On the other hand, β_l has a jump discontinuity at the wall.

Thus, the case which proves to be relevant for discussion of the generalized zeroth law is that in which the total action (for the composite system) is microcanonical and in which a jump discontinuity in the momentum variable β_l occurs at some surface where $\mathcal{E}_{\mathrm{B}}$ is continuous. To determine the contribution of such a jump discontinuity to the action, note

$$I_{\mathrm{M}} = -\int_0^1 \left(\beta\dot{\mathcal{E}}_{\mathrm{B}} + \ldots\right) + \lim_{\epsilon\to 0}\left\{\frac{1}{2}\int_{\alpha-\epsilon}^{\alpha+\epsilon} \frac{\partial}{\partial y}\left(\beta_l \mathcal{E}_{\mathrm{B}}\right) d^3x\, dy\right\}. \tag{7.5.8}$$

All terms in the first integrand have at most jump discontinuities at $y = \alpha$, so the contribution of the jump discontinuity is

$$I_{\mathrm{jump}} = \frac{1}{2}\int_{y=\alpha} \left(\beta_l|_+ - \beta_l|_-\right) \mathcal{E}_{\mathrm{B}}\, d^3x. \tag{7.5.9}$$

Include this contribution due to the jump discontinuity in β_l, to find that the *initial* total action for the composite system when two systems with different surface temperature come into thermal contact is just

$$I = I_1 + I_2 = -S_1 - S_2, \qquad (7.5.10)$$

where I_1 and I_2 are the actions associated with thermally isolated systems and are of the form given in (7.5.7). Note that the contribution of the jump discontinuity *is precisely that required to make entropy an extensive thermodynamic quantity.*

By definition, the diathermal wall allows for variations in energy at its surface. The final equilibrium configuration of the composite system must extremize the action subject to these variations. To see what this implies, vary the total action, integrate by parts and obtain,

$$\begin{aligned} \delta I &= -\frac{1}{16\pi}\int_0^{\alpha-} (G_{\mu\nu} - 8\pi T_{\mu\nu})\, \delta g^{\mu\nu}\, g^{1/2}\, d^3x\, dr \\ &- \frac{1}{16\pi}\int_{\alpha+}^{1} (G_{\mu\nu} - 8\pi T_{\mu\nu})\, \delta g^{\mu\nu}\, g^{1/2}\, d^3x\, dr + \int_{y=\alpha} \beta_l \big|_{\alpha-}^{\alpha+}\, \delta\mathcal{E}_B. \quad (7.5.11) \end{aligned}$$

If I is to be extremized under arbitrary variations, all three terms in (7.5.11) must vanish independently. The extremal metric will satisfy $G_{\mu\nu} = 8\pi T_{\mu\nu}$ in the regular regions, and also the surface equation,

$$\beta_l|_+ = \beta_l|_- \qquad (7.5.12)$$

at $y = \alpha$. In other words, a condition for extremizing the action is that the local temperature be continuous across the shared boundary. This 'generalized zeroth law of thermodynamics' can be viewed as a generalized Einstein equation which follows directly from the principle of least action.

There is an important difference between the classical zeroth law and the generalized zeroth law. The classical law suggests that when two systems are placed in thermal contact they evolve until they share a common temperature. The generalized zeroth law makes the weaker claim that the systems evolve until the local temperature is continuous across their shared boundary. It allows for the possibility of a stable temperature gradient in each system and even for a variation of local temperature over the surface of the shared boundary. The extra flexibility of the generalized zeroth law is entirely necessary if we are to allow for the stable temperature gradients that arise due to gravitational redshifting and blueshifting.

Also note, that equations (7.5.3) should be considered as generalized laws of thermodynamics analogous to the zeroth law. These equations imply that when two systems are separated by a surface which allows for arbitrary variations of the metric components h_{AB} (e.g. a flexible membrane), the values of π^{AB} will eventually become continuous across their shared boundary (e.g. they will come to a common surface pressure at the boundary).

7.6 The second law and the principle of least action

The second Law of classical thermodynamics may be formulated in a number of different ways. Notably, Clausius, Kelvin, and Carathéodory have each presented versions of the law. Except for possible subtleties of interpretation which can arise when one considers the interactions of non–equilibrium systems (see page 98 of Ref [20]), all these forms reduce to a simple statement:

The entropy of an isolated system can never diminish.

Here I propose that the generalized version of the second law of classical thermodynamics is the principle of least action. As was shown in Section 7.3, the classical action for an isolated system is equal to the negative of its entropy. The generalized second law might then be stated as follows[3];

> *The classical configuration of any isolated system will be the configuration of greatest entropy (least action) compatible with its boundary constraints.*

At first glance, this generalized second law seems a much stronger statement about nature than the classical requirement that $\Delta S \geq 0$ for isolated systems. Specifically, the generalized law stipulates that a system must be in the state of maximum entropy accessible to it whereas the classical law allows the system to be in any state so long as its entropy does not diminish over time.

On the other hand, even if one accepts that a system is always in the state of maximum entropy to which it has access, it is not clear that this implies $\Delta S \geq 0$ for an isolated system. It may be that one could alter the constraints on a system in such a way that the maximal entropy of the final state is less than the maximal entropy of the initial state, thus leading to a violation of the classical second law.

To see that the principle of least action does in fact imply $\Delta S \geq 0$, it is valuable to first review the significance of the classical second law.

Classical thermodynamic entropy is only defined for equilibrium systems. Since the entropy of an isolated system in equilibrium does not change, the second law is really meaningful only for transitions between initial and final equilibrium states.

An example of the classical second law at work occurs when one brings two initially isolated bodies into thermal contact. The second law stipulates that the

[3] After I completed this paper, Jim York has made me aware that he has had similar ideas on a generalized second law.

final combined entropy of the bodies cannot be less than it was initially. Essentially, what one does in this experiment is take an isolated system (the system of the two bodies taken as a whole) and relaxes an internal constraint of that system. Specifically, one relaxes a constraint on energy fluctuations at the surface of contact between the two bodies (by replacing an adiabatic wall by a diathermal one).

Another example of the second law at work occurs when one takes two initially isolated bodies and allows particle flow from one to another (e.g. puncture a canister of gas in a larger chamber). A third example occurs when one replaces a rigid wall separating two gas chambers with a flexible membrane to allow for fluctuations in volume. In each case, the experiment involves relaxing an internal constraint in an isolated system.

These considerations prompt Pippard to present the following formulation of the classical second law;

> *It is not possible to vary the constraints of an isolated system in such a way as to decrease the entropy.*

Now consider how the principle of least action applies to the first example of bringing two isolated bodies into thermal contact (for simplicity, imagine that one merely replaces an adiabatic wall separating the bodies by a diathermal one). Since each body is initially isolated, the microcanonical gravitational action applies and the body's initial classical action is equal to the negative of its entropy. If the temperatures of the two systems are not the same, a jump discontinuity in β_l occurs at the wall. The initial action (and entropy) of the composite system is just the sum of the actions (entropies) of the two bodies (see discussion of the zeroth law).

When the adiabatic wall is replaced by a diathermal one, variations of the energy are allowed across the wall and, with respect to the now larger class of allowed metrics, the initial action for the composite system is, in general, non-extremal. The principle of least action stipulates that the final equilibrium configuration will have the least possible action compatible with boundary constraints, hence,

$$\Delta I \leq 0 \qquad \text{and} \qquad \Delta S \geq 0. \tag{7.6.1}$$

In the general theory of isolated systems presented above, the constrained quantities are $\mathcal{E}, h_{0A}, h_{AB}$, and the particle number densities. Relaxing internal constraints on any of these quantities, in general, renders the initial action non-extremal. By the principle of least action, the entropy of the final configuration cannot be less than the entropy of the initial configuration.

A sketch proof that the principle of least action implies $\Delta S \geq 0$ for isolated systems is as follows. The classical (minimum) action of a system is determined by its boundary constraints. Hence, to alter the classical action, one must alter the constraints. This can only be accomplished by bringing the system into interaction with another system. Viewing the two systems as a single composite system, any interaction necessarily involves ***relaxation*** of the constraints on the composite system (because the sub-systems always retain the freedom not to interact). The classical action after relaxation of the constraint must be less than or equal to the action before relaxing the constraint. If the two systems are then taken out of contact with one another, the action does not change since the final boundary constraints at the surface of interaction remain the 'natural boundary' conditions imposed while the two systems were interacting. Since $\Delta I \leq 0$ for the operation, $\Delta S \geq 0$.

Finally, note that the generalized second law (i.e. principle of least action) yields the generalized zeroth law as a direct consequence. On the other hand, the zeroth law does not imply the second law. Recall that to obtain the generalized zeroth law it was sufficient to require only that the final equilibrium configuration *extremize* the action. The generalized second law stipulates the stronger condition that the final equilibrium state actually *minimize* the action.

7.7 The third law

The third law of classical thermodynamics, originally proposed by Nernst may be stated as follows;

The temperature of a system cannot be reduced to absolute zero in a finite series of operations.

I propose the following generalized third law of thermodynamics;

It is impossible to measure a local temperature of zero at the boundary of a system within a finite amount of time.

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The proof is as follows. Suppose an isolated system were to exist at zero temperature. Boundary conditions on the system must be adiabatic (otherwise the system would come into equilibrium with its finite temperature surroundings). At the boundary of the system, the variations of the classical action are (see discussion of the zeroth law)

$$\delta I\big|_{y=\alpha} = \int_{y=\alpha} \beta_l \big|_-^+ \delta \mathcal{E}\, d^3x. \tag{7.7.1}$$

If the isolated system is to be at zero temperature, $\beta_l|_{\alpha_-} = \infty$. On the other hand, $\beta_l|_{\alpha_+}$ is finite. Consequently, unless the energy of the boundary is specified with infinite precision, the variations of the action diverge and one cannot have anything approximating a classical configuration. However, by virtue of the uncertainty principle, $\Delta E \Delta t \geq \hbar$. So, if the energy of the system is specified with infinite precision, then the time required to make the zero temperature measurement is infinite. Thus, it is not possible to measure a system at zero temperature in a finite amount of time.

7.8 Summary

In this final chapter, I have generalized the results of the earlier chapters. I have presented the basis for a general theory of thermodynamics. This theory is based entirely on properties of the Euclidean action and its variations. The first law of thermodynamics expresses the variations of the classical action subject to variations of boundary data. Legendre transformations from one thermal ensemble to another reflect changes that must be made in the form of the action if it is to have a well defined variational principle subject to given boundary constraints. The zeroth law(s) of thermodynamics are essentially surface Einstein equations which, in the absence of matter shells, yield smoothness of the momenta as equilibrium conditions. The second law of thermodynamics is the principle of least action. The third law derives from a constraint imposed by the uncertainty principle on the possibility of measuring an infinite jump discontinuity in a momentum variable.

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APPENDIX A

THE HARTLE–HAWKING DERIVATION OF HORIZON TEMPERATURE

The Hartle–Hawking method (see Ref. [5] of Chapter 1) of deriving horizon thermal radiance is to examine the rate of particle emission from the horizon, then compare it with the rate of particle absorption, and demonstrate that the black hole is in a thermal 'vacuum' state at a temperature given by $T = \frac{\kappa}{2\pi}$.

For the sake of definiteness, assume that the background geometry is Schwarzschildean; the generalization to other background geometries is straightforward. The Schwarzschild metric, normalized so that $g_{00} \to -1$ as $r \to \infty$, is

$$ds^2 = -\left(1 - \frac{2M}{r}\right) dt^2 + \left(1 - \frac{2M}{r}\right)^{-1} dr^2 + r^2\, d\Omega^2, \tag{A.1}$$

where the parameter M can be identified with the mass of the black hole as measured at infinity and where $G = C = k = \hbar = 1$.

It is often convenient to express this metric in terms of null Kruskal coordinates, U and V,

$$ds^2 = -\left(32M^3 e^{-r/2M}/r\right) dU\, dV + r^2\, d\Omega^2, \tag{A.2}$$

where r is given implicitly by

$$UV = \left(1 - \frac{r}{2M}\right) e^{2\kappa r} \tag{A.3}$$

and κ is the surface gravity of the black hole given by

$$\kappa = \frac{1}{2}\frac{\partial}{\partial r}\left(1 - \frac{2M}{r}\right)\bigg|_{r=2M} = \frac{1}{4M}. \tag{A.4}$$

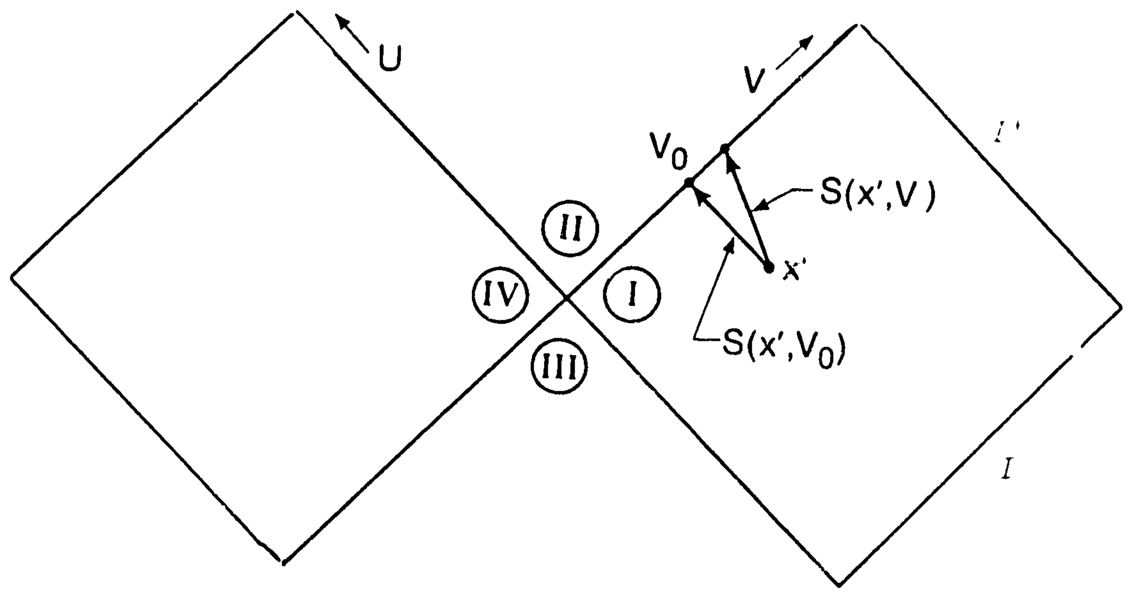

Figure A.1: Kruskal manifold for a Schwarzschild black hole. Region I is the physical sector, region II is the black hole interior, region III is the white hole interior and region IV is a 'shadow universe' causally disconnected from the physical universe. For an observer in region I, the future black hole horizon is the positive V axis; the past black hole horizon is the negative U axis. The surfaces $\mathcal{I}^+$ and $\mathcal{I}^-$ correspond to future and past null infinity respectively. The diagram shows a null geodesic from a point x' in region I to a point x_0 on the future horizon. A neighboring timelike geodesic has $V > V_0$ and $s(x, x') < 0$.

Figure A.1 represents the analytically continued Kruskal manifold. In this diagram, region I is the universe of an observer outside the black hole, region II is the black hole interior, region III is the white hole interior, and region IV is a 'shadow' universe with which physical observers have no contact. The black hole's past and future horizons are given respectively by the surfaces $V = 0$ and $U = 0$.

The transformations between the U, V and r, t coordinates in regions I and

II are

$$\left.\begin{aligned} U &= -\left(\frac{r}{2M}-1\right)^{1/2} e^{\kappa(r-t)} \\ V &= \left(\frac{r}{2M}-1\right)^{1/2} e^{\kappa(r+t)} \end{aligned}\right\} U<0,\ V>0 \text{ (region I)} \tag{A.5}$$

$$\left.\begin{aligned} U &= \left(1-\frac{r}{2M}\right)^{1/2} e^{\kappa(r-t)} \\ V &= \left(1-\frac{r}{2M}\right)^{1/2} e^{\kappa(r+t)} \end{aligned}\right\} U>0,\ V>0 \text{ (region II.)} \tag{A.6}$$

The transformations in regions IV and III are respectively the same as the above with the signs of U and V reversed.

Now consider the probability amplitude for particles to tunnel gravitationally from the black hole interior out to a physical observer. Let $G(x, x')$ be the amplitude for a scalar particle to propagate from the point x' to the point x. [Here x and x' each refer to four spacetime coordinates.] Then $G(x, x')$ is a solution of the inhomogeneous wave equation in the Schwarzschild background,

$$\left(\Box^2 - m^2\right) G(x, x') = -\delta(x, x'), \tag{A.7}$$

where $\Box^2 \equiv g^{ab}\nabla_a\nabla_b$ and ∇_a is covariant differentiation with respect to the Schwarzschild metric.

To specify the Green's function uniquely, choose a contour such that positive frequency modes are propagated forward in coordinate time t and negative frequency modes are propagated backward in t. For such a choice of contour, the appropriate Green's function is just the Feynman propagator,

$$G(x, x') = -\frac{i}{4\pi^2}\frac{1}{s(x, x') + i\varepsilon}, \tag{A.8}$$

where $s(x, x')$ denotes the square of the spacetime interval between x and x' and ε is a small positive constant with physical quantities being evaluated in the $\varepsilon \to 0$

limit. It is clear from (A.8) that the Feynman propagator has poles at $s(x, x') = -i\varepsilon$ corresponding to null geodesics from x' to x.

The Hartle–Hawking program is to define positive and negative frequency modes with respect to the past and future horizons. To this end, it is necessary to determine where the poles of the Feynman propagator lie on the complexified past and future horizons (the surfaces at which either one of U and V is equal to zero and the other extends over all complex values).

Consider then, a null geodesic extending from a point x' in sector I to a point x_0 on the future horizon. (See Figure A.1.) A singularity in $G(x, x')$ occurs on the complexified horizon at $V = V_1$ where V_1 is slightly displaced from V_0. For V close to V_0,

$$s(x, x') = \left(\frac{\partial s}{\partial V}\right)_{x_0} (V - V_0) + \ldots . \tag{A.9}$$

With $s(x_1, x') = -i\varepsilon$, equation (A.9) yields,

$$V_1 = V_0 - i\epsilon\left[\left(\frac{\partial s}{\partial V}\right)\bigg|_{V_0}\right]^{-1} . \tag{A.10}$$

To determine the sign of $\left(\frac{\partial s}{\partial V}\right)$ consider that a real timelike geodesic neighbouring the null geodesic from x' to x_0 has $s(x, x') < 0$ and $V > V_0$. Hence, by virtue of (A.9),

$$\left(\frac{\partial s}{\partial V}\right)_{x_0} < 0. \tag{A.11}$$

Now combine expressions (A.10) and (A.11) to see that the singularity of the propagator occurs in the upper half V plane.

By letting x' be a point in sector III and repeating the above analysis, one finds that the other singularity on the future horizon also lies above the real V axis. Thus, at $U = 0$, V is regular on the lower half plane.

To determine the domain of analyticity for the propagator on the complexified past horizon, one repeats the above analysis for a null geodesic emanating from a point x_0 on the past horizon to a point x' in region I. One finds that on the complexified past horizon the propagator has singularities in the lower half U plane and is analytic in the upper half U plane.

The analyticity properties of the Feynman propagator on the complexified horizon may be considered to define it as a particular solution of the inhomogeneous wave equation. From its behavior on the complexified horizon, it is possible to deduce the analytic properties of the propagator in all regions of the Kruskal manifold.

For instance, let us now return to the case in which x' is a point exterior to the black hole (ie. in region I) and x is a point in the black hole interior (ie. region II). The part of the future horizon with $V \geq 0$ and the section of the past horizon with $U \geq 0$ together form an initial Cauchy surface for region II. The propagator in this region is completely determined by the data on this Cauchy surface.

Furthermore, if one translates the temporal coordinate t of x to a complex value $t = \tau + i\sigma$, the analyticity properties of the propagator on the complexified horizon determine the analyticity properties of the translated propagator in the complexified region II. For a time translation of the form $t = \tau + i\sigma$, equations (A.6) yield,

$$\begin{aligned} U &= |U|e^{-i\sigma\kappa} \\ V &= |V|e^{i\sigma\kappa}. \end{aligned} \tag{A.12}$$

Since, $G_F(x, x')$ is analytic in the upper half U plane on $V = 0$ and the lower half

V plane on $U = 0$ the data (and hence solution) will be regular so long as

$$-\frac{\pi}{\kappa} \leq \sigma \leq 0 \tag{A.13}$$

Now suppose a particle detector is sensitive to particles of frequency ω. The relevant positive frequency mode emitted from the interior of the black hole will be proportional to $e^{-i\omega t}$. Hence, the amplitude for a scalar particle to propagate from a spacelike surface at fixed r to a point of detection outside the black hole at x' is proportional to

$$\mathcal{E}_\omega(\vec{R}', \vec{R}) = \int_{-\infty}^{\infty} e^{-i\omega t} G(0, \vec{R}'; t, \vec{R}) dt. \tag{A.14}$$

By virtue of the symmetry of $G(x, x')$ under interchange of x and x' this may also be written as

$$\mathcal{E}_\omega(\vec{R}', \vec{R}) = \int_{-\infty}^{\infty} e^{-i\omega t} G(t, \vec{R}; 0, \vec{R}';)dt. \tag{A.15}$$

The analyticity of $G_F(x, x')$ on the strip $-i\frac{\pi}{\kappa} < \text{Im}\ t < 0$ implies that the contour of integration may be displaced downward by $|\frac{\pi}{\kappa}|$,

$$\mathcal{E}_\omega(\vec{R}', \vec{R}) = e^{-\frac{\pi}{\kappa}\omega} \int_{-\infty}^{\infty} e^{-i\omega t} G_F(t - i\frac{\pi}{\kappa}, \vec{R}; 0, \vec{R}')\, dt \quad \text{for} \quad \kappa > 0. \tag{A.16}$$

By equations (A.5) and (A.6), the point

$$(t'', \vec{R}'') \equiv (t - i\frac{\pi}{\kappa}, \vec{R})$$

is the point in region III obtained by changing the sign of the U, V coordinates associated with $(t, \vec{R})$. Hence, the integral in (A.16) can be interpreted as the probability amplitude for a particle of frequency ω to be emitted from a spacelike surface of constant r in region III to a particle detector at $(0, \vec{R}')$. Further, by time-reversal invariance, this is equal to the probability amplitude for a particle to be emitted from the particle detector at $(0, \vec{R}')$ and *absorbed* by the black hole. Summing over the complete set of modes, the probability $\mathcal{P}_{\omega \text{ emission}}(\vec{R}', \vec{R})$ that the black hole will emit a particle of frequency ω is related to the probability $\mathcal{P}_{\omega \text{ absorption}}(\vec{R}', \vec{R})$ that the black hole will absorb a particle of the same frequency by

$$\mathcal{P}_{\omega \text{ emission}}(\vec{R}', \vec{R}) = e^{-2\pi\omega/\kappa} \times \mathcal{P}_{\omega \text{ absorption}}(\vec{R}', \vec{R}). \tag{A.17}$$

However, this relation between the emission and absorption probabilities characterizes particle radiance with a thermal spectrum of temperature

$$T = \frac{\kappa}{2\pi}. \tag{A.18}$$

Thus, one obtains the Hawking formula for horizon temperature.

APPENDIX B

THE ISRAEL DERIVATION OF HORIZON TEMPERATURE

A highly original method to obtain horizon temperature using Thermal Field Dynamics was devised by Israel in 1976 (see Ref. [6] of Chapter 1). Israel considers the generic stationary space–time described by the metric (1.2.1). Let

$$f_\omega(r,\theta,\phi,t) \propto \exp(-i\omega t) \tag{B.1}$$

be the energy eigenmodes of a Klein–Gordon field. Choose the time coordinate in equation (B.1) to correspond to the time measured by Killing observers. That is, advanced time along the V axis and retarded time along the U axis (see Figure B.1). For $U = 0$, the advanced time is $t = \frac{1}{\kappa}\ln|V|$. For $V = 0$, the retarded time is $t = -\frac{1}{\kappa}\ln|U|$.

Note that sectors I and IV are causally disjoint. Accordingly, associate with the eigenfunction f_ω Kruskal modes F_ω and $\tilde{F}_\omega$ where F_ω agrees with f_ω in sector I and is zero elsewhere, and where $\tilde{F}_\omega$ agrees with f_ω in sector IV and is zero elsewhere.

A field operator $\Phi(x)$ can then be expressed as

$$\Phi(x) = \sum_{\omega,j}\Big[a_{\omega j}F_{\omega j}(x) + \tilde{a}^\dagger_{\omega j}\tilde{F}_{\omega j}(x)\Big] \quad + \quad \text{h.c.} \tag{B.2}$$

where the index j is meant to span the complete set of eigenfunctions and $a^\dagger_{\omega j}$; $\tilde{a}^\dagger_{\omega j}$

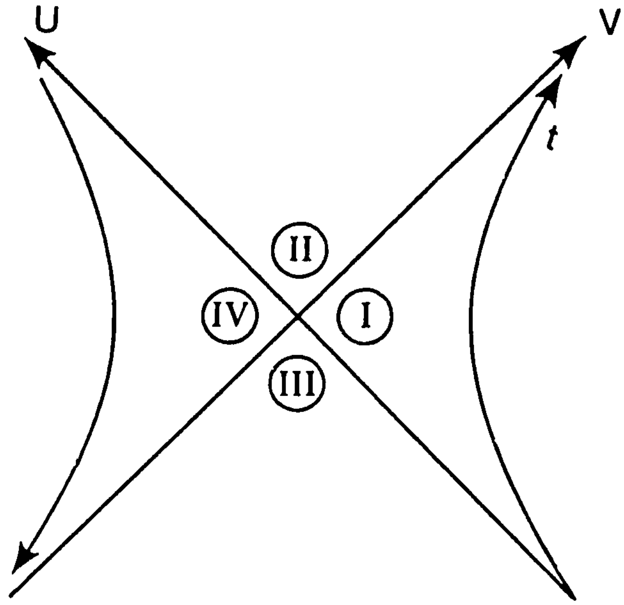

Figure B.1: Kruskal diagram for a static spherically symmetric vacuum metric. The surfaces $U = 0$ and $V = 0$ represent the past and future horizons respectively. The trajectories in region I and IV are the world lines of future directed Killing observers. Note that the time orientation of observers in region IV is opposite to that of observers in region I.

are creation operators obeying the commutation relations,

$$\left[a_{\omega i}, a^{\dagger}_{\omega' j}\right] = \left[\tilde{a}_{\omega i}, \tilde{a}^{\dagger}_{\omega' j}\right] = \delta_{ij}\delta(\omega - \omega') \tag{B.3}$$

$$\left[a_{\omega i}, \tilde{a}_{\omega' j}\right] = \left[a_{\omega i}, \tilde{a}^{\dagger}_{\omega' j}\right] = 0. \tag{B.4}$$

In the language of Thermal Field Dynamics, the $a_{\omega i}$ and $\tilde{a}^{\dagger}_{\omega i}$ operators create quasi-particle states; these states are not observable *per se*. The creation operator for observable particles can be obtained via a linear combination of the $a_{\omega i}$ and $\tilde{a}_{\omega i}$ which preserves the commutation relations (ie. via a Bogoliubov transformation). The general form of this transformation is

$$\begin{aligned} b_{\omega j} &= \cosh\phi_{\omega} a_{\omega j} - \sinh\phi_{\omega}\tilde{a}^{\dagger}_{\omega j} \\ \tilde{b}^{\dagger}_{\omega j} &= -\sinh\phi_{\omega} a_{\omega j} + \cosh\phi_{\omega}\tilde{a}^{\dagger}_{\omega j}, \end{aligned} \tag{B.5}$$

where $b^{\dagger}_{\omega j}$, $b_{\omega j}$ are the creation and annihilation operators associated with observable particles.

It is then possible to rexpress the field operator Φ as

$$\Phi = \sum_{\omega, j}\left[b_{\omega j}H_{\omega j}(x) + \tilde{b}^{\dagger}_{\omega j}\tilde{H}_{\omega j}(x)\right] \quad + \quad \text{h.c.}, \tag{B.6}$$

where

$$H_{\omega j} = \cosh\phi_{\omega}F_{\omega j} + \sinh\phi_{\omega}\tilde{F}_{\omega j} \tag{B.7}$$

$$\tilde{H}_{\omega j} = \sinh\phi_{\omega}F_{\omega j} + \cosh\phi_{\omega}\tilde{F}_{\omega j}. \tag{B.8}$$

Substituting into (B.7) the expressions for $F_{\omega j}, \tilde{F}_{\omega j}$ along the V axis,

$$H = \cosh\phi_{\omega} e^{-i\frac{\omega}{\kappa}\ln|V|}\theta(V) + \sinh\phi_{\omega} e^{-i\frac{\omega}{\kappa}\ln|V|}\theta(-V). \tag{B.9}$$

A function $f(t) \propto e^{-i\omega t}$ carries positive frequency with respect to t if and only if it is regular on the lower half complex t plane. Hence, choose a branch so that the logarithm function in (B.9) is regular on the lower half complex V plane. This choice yields for V real,

$$\ln(V) = \ln|V| - i\pi\theta(-V). \tag{B.10}$$

Now substitute into expression (B.9), to find that H is analytic in V if and only if

$$\tanh\phi_\omega = e^{-\frac{\pi}{\kappa}\omega}. \tag{B.11}$$

If one repeats the above analysis along the U axis, one also finds that H is analytic in U if and only if the above condition holds.

Now it is an axiom of Thermal Field Dynamics that the Bogoliubov parameter ϕ_ω is determined by

$$\tanh\phi_\omega = e^{-\frac{\beta\omega}{2}}, \tag{B.12}$$

where $\beta \equiv \frac{1}{T}$. Compare equations (B.11) and (B.12), to obtain the expected result

$$T = \frac{1}{2\pi}\kappa.$$

APPENDIX C

A BLACK HOLE IN THE MICROCANONICAL ENSEMBLE

To see how the properties of a system in the microcanonical ensemble relate to those in the canonical ensemble, consider the example of a Schwarzschild black hole in a box held at fixed energy and surface area. For such a system, equation (7.2.23) reduces to the York energy,

$$E = r_{\rm B}\left(1 - \left(1 - \frac{r_+}{r_{\rm B}}\right)^{1/2}\right), \tag{C.1}$$

and

$$\begin{aligned} I_{\rm M} &= -\pi r_+^2 \\ &= -\pi r_{\rm B}^2\left[1 - \left(1 - \frac{E}{r_{\rm B}}\right)^2\right]^2. \end{aligned} \tag{C.2}$$

By virtue of the Gibbons–Hawking relation between a classical action and free energy, equation (C.2) for $I_{\rm M}$ should have a thermodynamic interpretation. The 'free energy' appropriate to keeping the energy of the system fixed is obtained from the canonical free energy via a Legendre transformation,

$$\beta F_{\rm M} = \beta E - S - \beta E = -S, \tag{C.3}$$

where S is the entropy of the system. Identify $I_{\rm M}$ with $\beta F_{\rm M}$, to establish that the entropy of the black hole system is

$$S = \pi r_+^2. \tag{C.4}$$

Recalling that the weighting factor of the path integral is e^{-I}, it is clear that we have obtained a self consistent formulation of the gravitational microcanonical ensemble.

A system's thermodynamic properties in the microcanonical ensemble differ in some subtle ways from its thermodynamic properties in the canonical ensemble. For instance, recall that the canonical ensemble is not well defined for systems with negative heat capacity since the energy fluctuations for such systems would be imaginary. By contrast, the microcanonical ensemble can be well defined even for systems with negative heat capacity. [Energy fluctuations in the microcanonical ensemble are automatically zero since the internal energy is to be held fixed.]

Recall that in the canonical ensemble there are two black hole solutions which extremize the action with respect to the boundary data. By contrast, there is only one black hole solution which extremizes the action in the microcanonical canonical ensemble. To see this, note that r_+ is uniquely specified in terms of the boundary data by the equation,

$$r_+ = r_{\rm B}\left[1 - \left(1 - \frac{E_{\rm B}}{r_{\rm B}}\right)^2\right]. \tag{C.5}$$

The thermodynamic properties of the black hole in the microcanonical ensemble are easily derived. The inverse temperature of the black hole is defined by,

$$\begin{aligned}\beta &\equiv \left(\frac{\partial S}{\partial E_{\rm B}}\right)_{\rm A} \\ &= 4\pi r_{\rm B}\left(1 - \frac{E_{\rm B}}{r_{\rm B}}\right)\left(1 - \left(1 - \frac{E_{\rm B}}{r_{\rm B}}\right)^2\right).\end{aligned} \tag{C.6}$$

Expressed as a function of r_+ and $r_{\rm B}$, this expression agrees with the Hawking formula for the temperature of a Schwarzschild black hole. The microcanonical heat capacity of the black hole at fixed area is given by

$$\begin{aligned} C_A &= -\beta^2 \left(\frac{\partial E}{\partial \beta}\right) \\ &= \frac{\beta^2}{4\pi}\left[1 - 3\left(1 - \frac{E_B}{r_B}\right)^2\right]^{-1} . \end{aligned} \tag{C.7}$$

The black hole has positive heat capacity if

$$E_B > r_B \left(1 - \left(\frac{1}{3}\right)^{1/2}\right) . \tag{C.8}$$

Expressed in terms of r_+, this condition becomes

$$r_B < \frac{3}{2} r_+ , \tag{C.9}$$

which is the same as the condition for positive heat capacity in the canonical ensemble.

If $r_B > 3r_+/2$ the heat capacity of the black hole is negative. However, even for such cases, the black hole may be thermodynamically stable in the microcanonical ensemble. To determine whether or not such black holes are thermodynamically stable, one must explicitly incorporate the contribution to the action of the thermal radiation in the box and determine whether the black hole configuration locally maximizes the entropy of the system.

It is straightforward to generalize the above treatment to include the effects of a matter distribution or a cosmological horizon. Assuming the conserved particle numbers have been held fixed as is appropriate in the microcanonical ensemble, one finds by methods analogous to those used in Chapters 2 and 3, that for all such static, spherically symmetric systems the action is equal to the negative of the entropy.

APPENDIX D

THE PETIT ENSEMBLE AND BOUNDARY CONDITIONS FOR THE EARLY UNIVERSE

One might ask "Which set of boundary conditions is most realistic in a cosmological setting?" In particular, considering the issues raised in Chapter 6 surrounding primordial black hole nucleation, one might wonder what set of boundary conditions would approximate those of the early Universe.

For isolated, spherica mmetric black hole systems one has two sets of choices. First, one may fix either the energy of the system or its temperature. Second, one may fix either the system's surface area or its surface pressure.

Examine the first choice. To maintain a black hole system at constant energy, one would have to enclose it in a perfectly insulating shell. For real black holes, this seems a particularly unlikely condition to impose. On the other hand, cosmological conditions might arise in which a black hole is kept at a quasi-constant temperature. One might imagine, for instance, that primordial black holes in the very early Universe were kept at constant temperature by interaction with surrounding radiation. While it is true that the radiation will cool with Hubble expansion, it may be that, at least on relatively short time scales, a constant temperature approximation would be valuable.

The second choice is to fix either the surface area or the surface pressure of the black hole/box system. To fix the surface area of the system, one would have to enclose the black hole in a perfectly rigid box. It is difficult to imagine a cosmological setting that would approximate such a configuration. On the other hand, keeping a black hole system at constant surface pressure may be more plausible. Imagine a black hole surrounded by a flexible membrane kept at constant surface pressure by its interaction with external ambient radiation. This might reasonably approximate the conditions in the very early Universe as primordial black holes formed.

Consider then a black hole system kept at constant temperature and surface pressure. In this ensemble, the black hole horizon radius relates to the boundary data by the equation

$$0 = (8\pi\lambda - 2\pi/\beta)\, r_+^4 + r_+^3 - (\beta/4\pi)\, \frac{r_+^2}{2} - (\beta/4\pi)^2\, r_+ + \frac{1}{2}(\beta/4\pi)^3, \qquad \text{(D.1)}$$

where λ is the surface pressure of the system (see Section 3.2). From this, we see that there may be up to four black hole solutions which extremize the action subject to a set fixed temperature and surface pressure boundary conditions.

In all cases, the solutions have negative heat capacity (see Chapter 3). However, it is not clear what effect a matter distribution would have on the heat capacities of these solutions. Furthermore, it is not clear whether the sign of the heat capacity in this ensemble bears any relation to the thermodynamic stability of the solutions. Stable solutions minimize the free energy $F = E - TS + \lambda A$.

I have already intimated that this ensemble might be interesting from the viewpoint of analyzing primordial black hole formation in the very early Universe. The treatment of primordial black hole nucleation in Chapter 6 assumed that the temperature of the black holes nucleated was simply

$$T = \frac{1}{8\pi M}. \qquad \text{(D.2)}$$

While, as an order of magnitude estimate, this relation may be useful, it cannot be expected to hold for realistic conditions in the very early Universe. Furthermore, as stressed by York (see Ref. [15] of Chapter 1), black holes can only be expected to nucleate if their free energy is less than that of hot flat space. To determine whether black holes actually nucleate in the early Universe, one would have to compare their free energy with that of hot flat space.

Finally, note that there is a problem endemic to any treatment of black hole nucleation. When a black hole forms, a change in the topology occurs. However, the standard action path integral gives no information on how to weight different topologies. In fact, if the path integral is to be well defined, it is necessary to specify the topology of the manifold over which it is defined at the outset (see Chapter 4). To properly treat black hole nucleation, one would need to implement a theory of quantum topology.

APPENDIX E

COMPUTER PROGRAMS FOR CALCULATING BLACK HOLE DENSITIES IN THE EARLY UNIVERSE

The following programs were used to estimate primordial black hole densities in the very early Universe as part of the research reported in Chapter 6. In total, seven different programs were useful in the research.

The first program 'TCRIT' calculates the time at which the density of the black holes formed due to quantum gravitational tunneling equals the radiation energy density. It assumes that the black holes start evaporating immediately after forming. Densities are calculated starting at one Planck time. At this initial time, the entire energy of the Universe is assumed to be in the form of radiation. The results obtained using this program are collected in Table 6.1.

The second program 'BINRYEND' calculates a lower bound on the time at which the end of the binary phase should occur. It calculates the time at which condition (6.3.17) is satisfied. Different assumptions about the equilibrium ratio of black hole density to radiation energy density can be made by varying ALPHA which corresponds to the parameter α in the text. The results obtained using this program are reported as lower bounds on t_{end} in Table 6.2.

The third program 'ENDBIN; calculates an upper bound on the time at which the binary phase ends. It calculates the time at which the total mass of black holes within a comoving volume obtained using (6.3.16) decreases too rapidly to maintain the equilibrium ratio of black hole energy density to radiation energy density. Results obtained using this program are reported as upper bounds on t_{end} in Table 6.2.

The fourth program, 'SU5TCRIT', was designed specifically for application to the SU(5) model. If one assumes that black holes begin evaporating immediately after formation, then their energy density never becomes comparable to the energy density of the ambient radiation under the SU(5) model. Yet, it is possible that the black holes do not start evaporating immediately after forming. To resolve the question of when they begin to evaporate, one needs to know the equation of state for the Universe (ie. whether or not the black holes have a large enough energy density to significantly affect the evolution of the Universe). This program demonstrates that even if one assumes that the black hole do not evaporate at all, it is still safe to use the radiation dominate model until at least 10^3 Planck times.

The fifth and sixth programs—'TXTINT' and 'TXTINT2'—are also for use on the SU(5) model. They compare the time of interaction between black hole and ambient radiation with the dynamic time associated with Hubble expansion. TXTINT assumes immediate evaporation of the black holes. TXTINT2 assumes no black hole evaporation. Regardless which assumption is made, one finds that the initial dynamical time of Hubble expansion is less than the time of interaction. Hence, the only self consistent assumption is that the black holes begin evaporating immediately after forming.

The final program, 'RTIO-BH/RD', is also for use with the SU(5) model. It calculates the ratio of the black hole energy density to the radiation shown in

Figure 6.1.

```
      COMMON /BL1/PI,YTHETA,YGAM,YNUM
C     **************************************************************
C     *                         TCRIT                                *
C     *  This program is intended to find the time at which the     *
C     *  the density of black holes equals the radiation energy     *
C     *  density assuming evaporation begins immediately after      *
C     *  formation.  It assumes that the initial mass of the        *
C     *  black hole is equal to 1/(8*pi*T(rad)).                    *
C     *                                                              *
C     **************************************************************
      REAL T1,T2,PI,TCRIT,YGAM,YTHETA,YNUM,
     &ALPHA,ERRABS,ERRREL,RESULT,ERSULT
      EXTERNAL F,QDAGS
      ERRABS=0.0
      ERRREL=0.001
      PI=3.14159265
      READ(5,10) YNUM,YTHETA,ALPHA
 10   FORMAT(1X,F12.4,3X,F12.10,3X,F12.11)
      YGAM=1./(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &*YNUM))**.5))
      WRITE(6,12) YNUM,YTHETA,ALPHA,YGAM
 12   FORMAT(1X,F12.4,3X,F12.10,3X,F12.11,3X,F12.10)
      WRITE(6,15)
      DO 11 N=1,100
      T1=N/20.
      T2=(((8.*PI)**3)/(YNUM*3))*(.25*YGAM*T1/PI)**1.5+T1
      CALL QDAGS(F,T1,T2,ERRABS,ERRREL,RESULT,ERSULT)
      TCRIT=(36.*((1.-3.*ALPHA)**2)*(PI**4.))/(((RESULT*.87)**2.)
     &*((16.*PI*YGAM)**(YTHETA-1.)))
      WRITE (6,20)T2,TCRIT,RESULT,ERSULT
 11   CONTINUE
 15   FORMAT(3X,'TIME',8X,'TCRIT',7X,'RESULT',5X,'ERSULT')
 20   FORMAT(1X,F7.3,5X,F8.5,4X,F9.4,2X,F9.7)
      END
      REAL FUNCTION F (X)
      REAL X
      REAL EXP
      COMMON /BL1/PI,YTHETA,YGAM,YNUM
      F=(X**(1.+(YTHETA/2.)))*(((.25*(YGAM/PI)*X)**1.5+
     &(3.*YNUM/((8.*PI)**3))*(X-T2))**(1./3.))*EXP(-YGAM*X)
      RETURN
      END
```

```
      COMMON /BL1/T,PI,ALPHA,YGAM,YTHETA,YNUM
C     *************************************************************
C     *                      BINRYEND                             *
C     *  This program calculates a lower bound for the end time   *
C     *  of the binary phase.  It assumes that evaporation        *
C     *  of the black holes begins immediately after formation.   *
C     *  It calculates using double precision.                    *
C     *                                                           *
C     *************************************************************
      REAL*8 T,PI,ALPHA,YGAM,YTHETA
      REAL*8 ERRABS,ERRREL,RESULT,ERSULT,
     &Z,YNUM,TSTAR,TDENS1,TDENS2
      EXTERNAL F,DQDAGS
      ERRABS=0.0D0
      ERRREL=0.0001D0
      PI=3.14159265358979D0
      Z=1.D0
      READ(5,12) YNUM,YTHETA,ALPHA
 12   FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
 14   FORMAT(1X,F12.4,3X,F12.10,3X,F12.10,3X,F12.10)
      YGAM=1.D0/(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &*YNUM))**.5))
      WRITE(6,14) YNUM,YTHETA,ALPHA,YGAM
      WRITE(6,15)
      DO 10 N=1,100
      TSTAR=N/10.D0+1.D0
      T=(((8.*PI)**3)/(3.*YNUM))*(YGAM*TSTAR/(4.*PI))**1.5
     &+TSTAR
      TDENS2=(1.-3.*ALPHA)*2.*ALPHA*((8.*PI)**3)/(6.*PI*YNUM*
     &((1.+ALPHA)**3)*(T**((1.+3.*ALPHA)/(1.+ALPHA))))
      TDENS1=T**((2./(1.+ALPHA))+(YTHETA/2.))
     &*DEXP(-YGAM*T)*.5*((YGAM/PI)**.5)*((8.*PI)**3)/YNUM
     &+TDENS2
      CALL DQDAGS(F,TSTAR,T,ERRABS,ERRREL,RESULT,ERSULT)
      WRITE (6,20)T,TSTAR,RESULT,ERSULT,TDENS1,TDENS2
 10   CONTINUE
 15   FORMAT(3X,'UPLIM',4X,'LOLIM',5X,
     &'RESULT',4X,'ERSULT',5X,
     &'TDENS1',7X,'TDENS2')
 20   FORMAT(1X,F7.1,2X,F7.4,2X,E11.4,2X,F8.5,2X,E11.4,2X,E11.4)
      END
      REAL FUNCTION F*8 (X)
      COMMON /BL1/T,PI,ALPHA,YGAM,YTHETA,YNUM
      REAL*8 T,PI,ALPHA,YGAM,YTHETA,YNUM
      REAL*8 X
      F=(((.25*(YGAM/PI)*X)**1.5+3.*(YNUM/((8.*PI)**3))
     &*(X-T))**(-2.D0/3.D0))
     &*(X**((2./(1.+ALPHA))-.5+(YTHETA/2.)))*DEXP(-YGAM*X)
      RETURN
      END
```

```
      COMMON /BL1/T,TPLUS,PI,ALPHA,YGAM,YTHETA,YNUM
C     ***********************************************************
C     *                          ENDBIN                         *
C     *  This program calculates the end time of the            *
C     *  binary phase.  It assumes that evaporation             *
C     *  of the black holes begins immediately after formation. *
C     *  It is calculated using double precision.               *
C     *  To calculate the end time, we compare the decrease in  *
C     *  the mass of black holes within a comoving volume       *
C     *  (calculated using the formula of GPY and integrating   *
C     *  from T to TPLUS) with the decrease in mass of black    *
C     *  holes within a comoving volume calculated with the     *
C     *  the solution between T and TPLUS                       *
C     *                                                         *
C     ***********************************************************
      REAL*8 T,TPLUS,PI,ALPHA,YGAM,YTHETA
      REAL*8 ERRABS,ERRREL,RESULT,ERSULT,
     &Z,YNUM,TDELM1
      EXTERNAL F,DQDAGS
      ERRABS=0.0D0
      ERRREL=0.0001D0
      PI=3.14159265358979D0
      Z=1.D0
      READ(5,12) YNUM,YTHETA,ALPHA
   12 FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
   14 FORMAT(1X,F12.4,3X,F12.10,3X,F12.10,3X,F12.10)
      YGAM=1.D0/(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &*YNUM))**.5))
      WRITE(6,14) YNUM,YTHETA,ALPHA,YGAM
      WRITE(6,15)
      DO 10 N=8,100
      T=N*1.D0
      TPLUS=T+1.
      TDELM1=(1-3*ALPHA)/(3*PI*((1+ALPHA)**2)*(T**3))
C      Note that upper and lower limits of integration
C      are inverted to account for the anticipated negative
C      change in total mass within the comoving volume.
      CALL DQDAGS(F,TPLUS,T,ERRABS,ERRREL,RESULT,ERSULT)
      WRITE (6,20)TPLUS,T,RESULT,ERSULT,TDELM1
   10 CONTINUE
   15 FORMAT(3X,'UPLIM',4X,'LOLIM',5X,
     &'RESULT',4X,'ERSULT',5X,
     &'TDELM1')
   20 FORMAT(1X,F7.1,2X,F7.4,2X,E11.4,2X,F8.5,2X,E11.4)
      END
      REAL FUNCTION F*8 (X)
      COMMON /BL1/T,TPLUS,PI,ALPHA,YGAM,YTHETA,YNUM
      REAL*8 T,TPLUS,PI,ALPHA,YGAM,YTHETA,YNUM
      REAL*8 X
      F=(((.25*(YGAM/PI)*X)**1.5+3.*(YNUM/((8.*PI)**3))
     &*(X-TPLUS))**(1.D0/3.D0))
     &*(X**((2./(1.+ALPHA))-.5+(YTHETA/2.)))*DEXP(-YGAM*X)
      RETURN
      END
```

```
      COMMON /BL1/PI,YTHETA,YGAM,YNUM
C     ***********************************************************
C     *                        SUBTCRIT                         *
C     *  This program is designed specifically for finding the  *
C     *  time at which the density of black holes equals beta   *
C     *  times the density of ambient radiation.  It assumes no *
C     *  evaporation. and that the initial mass of the          *
C     *  black hole is equal to 1/(8*pi*T(rad)).                *
C     *                                                         *
C     ***********************************************************
      REAL T1,T2,PI,TCRIT,YGAM,YTHETA,YNUM,
     &ALPHA,ERRABS,ERRREL,RESULT,ERSULT
      EXTERNAL F,QDAGS
      ERRABS=0.0
      ERRREL=0.001
      PI=3.14159265
      READ(5,10) YNUM,YTHETA,ALPHA
10    FORMAT(1X,F12.4,3X,F12.10,3X,F12.11)
      YGAM=1./(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &*YNUM))**.5))
      WRITE(6,12) YNUM,YTHETA,ALPHA,YGAM
12    FORMAT(1X,F12.4,3X,F12.10,3X,F12.11,3X,F12.10)
      WRITE(6,15)
      DO 11 N=1,20
      T1=1.
      T2=2.*N
      CALL QDAGS(F,T1,T2,ERRABS,ERRREL,RESULT,ERSULT)
      TCRIT=(36.*((1.-3.*ALPHA)**2)*(PI**4.))/(((RESULT*.87)**2.)
     &*((16.*PI*YGAM)**(YTHETA-1.)))
      WRITE (6,20)T2,TCRIT,RESULT,ERSULT
11    CONTINUE
15    FORMAT(3X,'TIME',8X,'TCRIT',7X,'RESULT',5X,'ERSULT')
20    FORMAT(1X,F7.3,5X,F12.1,4X,F9.4,2X,F9.7)
      END
      REAL FUNCTION F (X)
      REAL X
      REAL EXP
      COMMON /BL1/PI,YTHETA,YGAM,YNUM
      F=(X**(1.+(YTHETA/2.)))*((.25*(YGAM/PI)*X)**.5)
     &*EXP(-YGAM*X)
      RETURN
      END
```

```
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
C ****************************************************************
C *                          TXTINT                               *
C *   This program compares the interaction time between black    *
C *   holes and ambient radiation with the dynamic time of        *
C *   expansion.  It assumes immediate evaporation of the black   *
C *   holes.                                                      *
C *                                                               *
C ****************************************************************
      REAL T1,YNUM,T2,TXP,PI,TINT,
     &ERRABS,ERRREL,RESLT1,ERSLT1,RESLT2,ERSLT2
      EXTERNAL F,F2,QDAGS
      ERRABS=0.0
      ERRREL=0.001
      PI=3.14159265
      READ(5,10) YNUM,YTHETA,ALPHA
      YGAM=1./(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &*YNUM))**.5))
10    FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
      WRITE(6,12) YNUM,YTHETA,ALPHA,YGAM
12    FORMAT(1X,F12.4,3X,F12.10,3X,F12.10,3X,F12.10)
      WRITE(6,15)
      DO 11 N=1,100
      T1=N/2.
      T2=(((8.*PI)**3)/(YNUM*3))*(.25*YGAM*T1/PI)**1.5+T1
      CALL QDAGS(F,T1,T2,ERRABS,ERRREL,RESLT1,ERSLT1)
      CALL QDAGS(F2,T1,T2,ERRABS,ERRREL,RESLT2,ERSLT2)
      TINT=(RESLT2*16.*PI*PI*(T2**1.5))/((RESLT1**2.)
     &*9*.87*((16.*PI*YGAM)**(.5*(YTHETA-1.))))
      TXP=3.*T2**(1+ALPHA)*.5
      WRITE (6,20)TXP,TINT,RESLT1,ERSLT1,RESLT2,ERSLT2
11    CONTINUE
15    FORMAT(3X,'TEXP',4X,'TINT',4X,'RESLT1',5X,'ERSLT1'
     &,5X,'RESLT2',5X,'ERSLT2')
20    FORMAT(1X,F5.1,5X,F5.1,4X,F5.2,2X,F9.7,4X,F5.2,2X,F9.7)
      END
      REAL FUNCTION F (X)
      REAL X
      REAL EXP
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
      F=(X**((2./(1.+ALPHA))-.5+(YTHETA/2.)))
     &*((((.25*(YGAM/PI)*X)**1.5)+3.*(YNUM/(8.*PI)**3)
     &*(X-T2))**(1./3))*EXP(-YGAM*X)
      RETURN
      END
      REAL FUNCTION F2 (Y)
      REAL Y
      REAL EXP
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
      F2=(Y**((2./(1.+ALPHA))-.5+(YTHETA/2.)))
     &*EXP(-YGAM*Y)
      RETURN
      END
```

```fortran
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
C     ******************************************************
C     *                     TXTINT2                          *
C     *  This program compares the time of interaction       *
C     *  between black holes and radiation with the time of *
C     *  expansion associated with the binary model.         *
C     *  It assumes that no evaporation takes place          *
C     *                                                      *
C     ******************************************************
      REAL T1,YNUM,T2,TXP,PI,TINT,
     &ERRABS,ERRREL,RESLT1,ERSLT1,RESLT2,ERSLT2
      EXTERNAL F,F2,QDAGS
      ERRABS=0.0
      ERRREL=0.001
      PI=3.14159265
      READ(5,10) YNUM,YTHETA,ALPHA
      YGAM=1./(16.*PI*((5./((PI**3)*((1.+ALPHA)**2)
     &+YNUM))**.5))
   10 FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
      WRITE(6,12) YNUM,YTHETA,ALPHA,YGAM
   12 FORMAT(1X,F12.4,3X,F12.10,3X,F12.10,3X,F12.10)
      WRITE(6,15)
      DO 11 N=1,100
      T1=1.
      T2=N*1.+1.
      CALL QDAGS(F,T1,T2,ERRABS,ERRREL,RESLT1,ERSLT1)
      CALL QDAGS(F2,T1,T2,ERRABS,ERRREL,RESLT2,ERSLT2)
      TINT=(RESLT2*16.*PI*PI*(T2**1.5))/((RESLT1**2.)
     &*9*.87*((16.*PI*YGAM)**(.5*(YTHETA-1.))))
      TXP=3.*T2*(1+ALPHA)*.5
      WRITE (6,20)TXP,TINT,RESLT1,ERSLT1,RESLT2,ERSLT2
   11 CONTINUE
   15 FORMAT(3X,'TEXP',4X,'TINT',4X,'RESLT1',5X,'ERSLT1'
     &,5X,'RESLT2',5X,'ERSLT2')
   20 FORMAT(1X,F5.1,5X,F5.1,4X,F5.2,2X,F9.7,4X,F5.2,2X,F9.7)
      END
      REAL FUNCTION F (X)
      REAL X
      REAL EXP
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
      F=(X**((2./(1.+ALPHA))-.5+(YTHETA/2.)))
     &*(.25*(YGAM/PI)*X)**.5
     &*EXP(-YGAM*X)
      RETURN
      END
      REAL FUNCTION F2 (Y)
      REAL Y
      REAL EXP
      COMMON /BL1/YNUM,ALPHA,T2,PI,YTHETA,YGAM
      F2=(Y**((2./(1.+ALPHA))-.5+(YTHETA/2.)))
     &*EXP(-YGAM*Y)
      RETURN
      END
```

```
      COMMON /BL1/T2,PI,YTHETA,YGAM
C ********************************************************************
C *                          RTIO-BH/RAD                             *
C *  This program is used to calculate the ratio of the black        *
C *  energy density to the radiation energy density as a             *
C *  function of time.  It assumes that black holes begin            *
C *  evaporating immediately after formation.                        *
C *  It also assumes a radiation dominated model.                    *
C *                                                                  *
C ********************************************************************
      REAL TSTAR,T2,PI,TFRAC,
     &ERRABS,ERRREL,RESULT,ERSULT
      EXTERNAL F,QDAGS
      ERRABS=0.0
      ERRREL=0.001
      PI=3.14159265
      READ(5,10) YNUM,YTHETA
 10   FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
      YGAM=1./(16.*PI*((5./((PI**3)*((4./3.)**2)
     &*YNUM))**.5))
      WRITE(6,12) YNUM,YTHETA,YGAM
 12   FORMAT(1X,F12.4,3X,F12.10,3X,F12.10)
      WRITE(6,15)
      TSTAR=.8
      DO 11 N=10,110
      TSTAR=TSTAR+.2
      T2=(((8.*PI)**3)/(3.*YNUM))*(YGAM*TSTAR/(4.*PI))**1.5
     &+TSTAR
      CALL QDAGS(F,TSTAR,T2,ERRABS,ERRREL,RESULT,ERSULT)
      TFRAC=(6.*(PI**2))/(RESULT*.87*((16.*PI*YGAM)**
     &((YTHETA-1.)/2.))*(T2**.5))
      TFRAC=1./TFRAC
      WRITE (6,20)T2,TFRAC,TSTAR
 11   CONTINUE
 15   FORMAT(2X,'TIME',8X,'BH/RAD',6X,'TSTAR')
 20   FORMAT(1X,F7.3,4X,F9.6,4X,F7.3)
      END
      REAL FUNCTION F (X)
      REAL X
      REAL EXP
      COMMON /BL1/T2,PI,YTHETA,YGAM
      F=(((.25*(YGAM/PI)*X)**1.5+3.*(YNUM/((8.*PI)**3))
     &*(X-TPLUS))**(1./3.))
     &*(X**(1.+(YTHETA/2.)))*EXP(-YGAM*X)
      RETURN
      END
```