Hamiltonian thermodynamics of the Schwarzschild black hole

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Kuchař has recently given a detailed analysis of the classical and quantum geometrodynamics of the Kruskal extension of the Schwarzschild black hole. In this paper we adapt Kuchař's analysis to the exterior region of a Schwarzschild black hole with a timelike boundary. The reduced Lorentzian Hamiltonian is shown to contain two independent terms: one from the timelike boundary and the other from the bifurcation two-sphere. After quantizing the theory, a thermodynamical partition function is obtained by analytically continuing the Lorentzian time evolution operator to imaginary time and taking the trace. This partition function is in agreement with the partition function obtained from the Euclidean path integral method; in particular, the bifurcation two-sphere term in the Lorentzian Hamiltonian gives rise to the black hole entropy in a way that is related to the Euclidean variational problem. We also outline how Kuchař's analysis of the Kruskal spacetime can be adapted to the $\mathbb{R}P^3$ geon, which is a maximal extension of the Schwarzschild black hole with $\mathbb{R}P^3 \setminus \{p\}$ spatial topology and just one asymptotically flat region.

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I. INTRODUCTION

In the path integral approach to black hole thermodynamics, one wishes to compute the partition function of a thermodynamical ensemble containing a black hole from a path integral of the form $\int \mathcal{D}g_{ab} \exp(iS)$ or $\int \mathcal{D}g_{ab} \exp(-I)$, subject to an appropriate set of boundary conditions. The initial impetus for this approach came in the observation [1,2] that for the Kerr-Newman family of black holes in asymptotically flat space, a saddle point estimate for the path integral yields a partition function which reproduces the black hole entropy that was first obtained by combining Hawking's result of black hole radiation [3] with the dynamical laws of classical black hole geometries [4] in the manner anticipated by Bekenstein [5,6]. The subject has since evolved considerably; see, for example, Refs. [7–13].

Given the progress made within the path integral approach, one is inclined to ask to what extent similar thermodynamical partition functions could be derived by starting from a Lorentzian Hamiltonian quantum theory of black holes, in a way more closely analogous to what is done in flat space thermal field theory. Consider in particular a quantum black hole with boundary conditions that fix the temperature, so that the thermodynamics is described by the canonical ensemble [14]. Does there exist a Lorentzian quantum theory, with a Hamiltonian operator $\hat{\mathbf{h}}$ acting on some appropriate Hilbert space, such that one can obtain a thermodynamical partition function by analytically continuing the time evolution operator and then taking the trace? Most importantly, does such a partition function agree with the one obtained from the path integral approach, at least in the semiclassical approximation?

One can argue that a necessary condition for the existence of a Lorentzian quantum theory of this kind is that the heat capacity of the system be positive. In other words, the canonical ensemble must be thermodynamically stable. Suppose that the Lorentzian quantum theory leads to an expression for the partition function in the form

$$Z(\beta) = \mathrm{Tr} \exp(-\beta \hat{\mathbf{h}}) \quad , \tag{1.1}$$

where $\hat{\mathbf{h}}$ is the quantum Hamiltonian and β the inverse temperature. Taking the trace in the energy eigenstate basis gives $Z(\beta)$ in the form of a Laplace transform:

$$Z(\beta) = \int dE\, \nu(E) \exp(-\beta E) \quad , \tag{1.2}$$

where $\nu(E)$ is the density of states associated with $\hat{\mathbf{h}}$ [15,16]. $\nu(E)$ may in general be either an ordinary function, corresponding to a continuous spectrum, or a sum of δ functions, corresponding to a discrete spectrum, or a combination of the two. Assuming that $\nu(E)$ is nonnegative and the integral in (1.2) converges, it follows by straightforward manipulations that the heat capacity $C = \beta^2 (\partial^2 (\ln Z)/\partial \beta^2)$ cannot be negative.

It is well known that Kerr-Newman black holes in asymptotically flat space are thermodynamically unstable for small values of charge and angular momentum [17,18]. However, one can achieve stability by replacing

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asymptotic flatness with other kinds of boundary conditions [7,10,15,19–24].[1] A simple example is obtained by placing a Schwarzschild black hole at the center of a mechanically rigid spherical box, with the temperature at the box fixed [15]. This boxed Schwarzschild system will be the focus of the present paper. We shall present a Lorentzian quantum theory from which a thermodynamical partition function can be obtained as the trace of the time evolution operator that has been analytically continued to imaginary time. When the continuation is done suitably, this partition function is in agreement with the one obtained from the Euclidean path integral approach in Refs. [15,16,28–31].

By Birkhoff's theorem [32], one might not anticipate that spherically symmetric pure gravity could be cast in the form of an unconstrained Hamiltonian system. From the spacetime point of view the solution space is one dimensional, parametrized by the Schwarzschild mass: This solution space is clearly not a phase space. However, it was demonstrated recently [33–36] that a Hamiltonian reduction of spherically symmetric gravity under certain types of boundary conditions does lead to a canonical *pair* of unconstrained degrees of freedom. One member of the pair can be chosen to be the Schwarzschild mass, and its conjugate momentum is related to the boundary conditions that one adopts at the ends of the spacelike hypersurfaces. These results raise the possibility of obtaining a Hamiltonian description also for a Schwarzschild hole in a finite box.

The Hamiltonian analysis of Kuchař [36] was performed under boundary conditions appropriate for the full Kruskal spacetime, with the spatial slices extending from one spatial infinity to the other and crossing the horizons in arbitrary ways. In the present paper we modify these boundary conditions in two respects. First, we replace the right-hand-side spatial infinity by a timelike three-surface in the right-hand-side exterior Schwarzschild region. This timelike three-surface is viewed as the "box" whose intrinsic metric will be fixed in the variational analysis. Second, we replace the left-hand-side spatial infinity by the horizon bifurcation two-sphere, where the past and future horizons cross: The spatial slices are required to approach the bifurcation two-sphere in a way asymptotic to surfaces of constant Killing time. The spatial slices are thus entirely contained within the right-hand-side exterior region of the Kruskal spacetime. It will be seen that a Hamiltonian reduction under these boundary conditions leads again to a canonical pair of unconstrained degrees of freedom, with one member of the pair being the Schwarzschild mass, and its conjugate momentum being related to the boundary conditions at the two ends of the spatial slices. We exhibit in particular a reduced Hamiltonian formulation where the quantities specifying the evolution of the left and right ends of the spatial slices appear as independent, prescribed parameters in the true Hamiltonian.

After specializing to the case where the radius of the "box" is time independent, we canonically quantize the reduced Hamiltonian theory in a straightforward manner. The time evolution operator $\hat{K}$ of the quantum theory turns out to contain not just one but two evolution parameters: The operator is of the form $\hat{K}(T_B, \Theta_H)$, where T_B is the proper time elapsed at the timelike boundary and Θ_H is the "boost parameter" elapsed at the bifurcation two-sphere. It will be shown that the expression

$$Z(\beta) = \mathrm{Tr}\left[\hat{K}(-i\beta; -2\pi i)\right] \quad , \tag{1.3}$$

when appropriately renormalized, yields a partition function that is in agreement with the one derived from the Euclidean path integral approach in Refs. [15,16,28–31]. The choice of the first argument of $\hat{K}$ on the right hand side of (1.3) follows from interpreting β as the inverse temperature measured at the boundary. The choice of the second argument of $\hat{K}$ is made so that the classical solutions to the reduced Hamiltonian theory with the boundary data of (1.3) are the Euclidean (or complex) Schwarzschild solutions that appear as saddle points in the Euclidean path integral approach. This choice of the second argument of $\hat{K}$ is analogous to choosing the four-manifold in the Euclidean path integral approach to be the one admitting the Euclidean Schwarzschild solution.

The plan of the paper is as follows. In Sec. II we set up the Hamiltonian description of spherically symmetric gravity under our boundary conditions in the conventional metric [Arnowitt-Desner-Misner (ADM)] variables. In Sec. III we adapt the canonical transformation of Kuchař to our boundary conditions, and in Sec. IV the theory is reduced to an unconstrained Hamiltonian form in which quantities specifying the evolution at the two ends of the spatial slices appear as parameters in the true Hamiltonian. The quantum theory is constructed and the partition function (1.3) analyzed in Sec. V. The results are summarized and discussed in Sec. VI. Appendix A addresses the regularization and renormalization of the trace in (1.3). In Appendixes B and C we outline how the geometrodynamical analysis of Kuchař can be adapted from Kruskal boundary conditions to boundary conditions appropriate for the $\mathbb{R}P^3$ geon [37], which is a maximal extension of the Schwarzschild black hole with $\mathbb{R}P^3 \setminus \{p\}$ spatial topology and just one asymptotically flat region.

Because of the nature of the work, we will often need to use results from Kuchař with little or no modification. We have aimed at a presentation that would remain self-contained in broad outline, while referring to Kuchař for some of the more technical details.

II. METRIC FORMULATION

In this section we shall set up the Hamiltonian formulation appropriate for our boundary conditions. The notation follows that of Kuchař.

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[1] Achieving not only thermodynamical but also mechanical stability in such systems remains nevertheless a subtle issue [7,25–27].

Our starting point is the general spherically symmetric spacetime metric on the manifold $\mathbb{R}\times\mathbb{R}\times S^2$, written in the ADM form as

$$ds^2 = -N^2dt^2 + \Lambda^2(dr + N^r dt)^2 + R^2 d\Omega^2 \quad . \tag{2.1}$$

Here $d\Omega^2$ is the metric on the unit two-sphere, and N, N^r, Λ, and R are functions of t and r only. We shall be interested in boundary conditions under which the radial proper distance $\int \Lambda\, dr$ on the constant t surfaces is finite. To impose this it is convenient to take the radial coordinate r to have a finite range, which can without loss of generality be chosen to be $[0,1]$. Unless otherwise stated, we shall throughout assume both the spatial metric and the spacetime metric to be nondegenerate. In particular, we take Λ, R, and N to be positive. We shall work in natural units, that is, with $\hbar = c = G = 1$.

The Einstein-Hilbert action for the metric (2.1) reads, up to boundary terms,

$$\begin{aligned} S_\Sigma[R,\Lambda;N,N^r] = \int dt \int_0^1 dr\, \big(&-N^{-1}\{R[-\dot\Lambda + (\Lambda N^r)'] \\ &\times(-\dot R + R'N^r) + \tfrac12\Lambda(-\dot R + R'N^r)^2\} \\ &+N(-\Lambda^{-1}RR'' + \Lambda^{-2}RR'\Lambda' \\ &-\tfrac12\Lambda^{-1}R'^2 + \tfrac12\Lambda)\big) \quad . \end{aligned} \tag{2.2}$$

The equations of motion derived from (2.2) are the full Einstein equations for the metric (2.1), and they imply that every classical solution is part of a maximally extended Schwarzschild spacetime, where the value of the Schwarzschild mass may be positive, negative, or zero. We shall discuss the boundary conditions and the boundary terms after passing to the Hamiltonian formulation.

From the Lagrangian action (2.2), the momenta conjugate to Λ and R are found to be

$$P_\Lambda = -N^{-1}R\left(\dot R - R'N^r\right) \quad , \tag{2.3a}$$

$$P_R = -N^{-1}\{\Lambda(\dot R - R'N^r) + R[\dot\Lambda - (\Lambda N^r)']\}. \tag{2.3b}$$

A Legendre transformation leads to the Hamiltonian action

$$\begin{aligned} &S_\Sigma[\Lambda, R, P_\Lambda, P_R; N, N^r] \\ &\quad = \int dt \int_0^1 dr (P_\Lambda\dot\Lambda + P_R\dot R - NH - N^rH_r) \quad , \end{aligned} \tag{2.4}$$

where the super-Hamiltonian H and the radial supermomentum H_r are given by

$$\begin{aligned} H = &-R^{-1}P_RP_\Lambda + \tfrac12 R^{-2}\Lambda P_\Lambda^2 + \Lambda^{-1}RR'' \\ &-\Lambda^{-2}RR'\Lambda' + \tfrac12\Lambda^{-1}R'^2 - \tfrac12\Lambda \quad , \end{aligned} \tag{2.5a}$$

$$H_r = P_RR' - \Lambda P_\Lambda' \quad . \tag{2.5b}$$

The Poisson brackets of the constraints close according to the radial version of the Dirac algebra [38].

We now turn to the boundary conditions. At $r \to 0$, we adopt the falloff conditions

$$\Lambda(t,r) = \Lambda_0(t) + O(r^2) \quad , \tag{2.6a}$$

$$R(t,r) = R_0(t) + R_2(t)r^2 + O(r^4) \quad , \tag{2.6b}$$

$$P_\Lambda(t,r) = O(r^3) \quad , \tag{2.6c}$$

$$P_R(t,r) = O(r) \quad , \tag{2.6d}$$

$$N(t,r) = N_1(t)r + O(r^3) \quad , \tag{2.6e}$$

$$N^r(t,r) = N^r_1(t)r + O(r^3) \quad , \tag{2.6f}$$

where Λ_0 and R_0 are positive, and $N_1 \geq 0$. Here $O(r^n)$ stands for a term whose magnitude at $r \to 0$ is bounded by r^n times a constant, and whose kth derivative at $r \to 0$ is similarly bounded by r^{n-k} times a constant for $1 \leq k \leq n$. It is straightforward to verify that the conditions (2.6) are consistent with the equations of motion: Provided the constraints $H = 0 = H^r$ and the falloff conditions (2.6a)–(2.6d) hold for the initial data, and provided the lapse and shift satisfy (2.6e) and (2.6f), it then follows that the falloff conditions (2.6a)–(2.6d) are preserved in time by the time evolution equations.[2] Equations (2.6a) and (2.6b) imply that the classical solutions have a positive value of the Schwarzschild mass, and that the constant t slices at $r \to 0$ are asymptotic to surfaces of constant Killing time in the right-hand-side exterior region in the Kruskal spacetime, all approaching the bifurcation two-sphere as $r \to 0$. The spacetime metric has thus a coordinate singularity at $r \to 0$, but this singularity is quite precisely controlled. In particular, in a classical solution the future unit normal to a constant t surface defines at $r \to 0$ a future timelike unit vector $n^a(t)$ at the bifurcation two-sphere of the Kruskal spacetime, and the evolution of the constant t surfaces boosts this vector at the rate given by

$$n^a(t_1)n_a(t_2) = -\cosh\left(\int_{t_1}^{t_2} \Lambda_0^{-1}(t)N_1(t)\,dt\right) \quad . \tag{2.7}$$

At $r = 1$, we fix R and $-g_{tt} = N^2 - (\Lambda N^r)^2$ to be prescribed positive-valued functions of t. This means fixing the metric on the three-surface $r = 1$, and in particular fixing this metric to be timelike. In the classical solutions, the surface $r = 1$ is located in the right-hand-side exterior region of the Kruskal spacetime.

We now wish to give an action principle appropriate for these boundary conditions. A first observation is that the surface action $S_\Sigma[\Lambda, R, P_\Lambda, P_R; N, N^r]$ [Eq. (2.4)] is well defined under the above conditions. Consider the total action

$$\begin{aligned} S[\Lambda, R, P_\Lambda, P_R; N, N^r] &= S_\Sigma[\Lambda, R, P_\Lambda, P_R; N, N^r] \\ &\quad + S_{\partial\Sigma}[\Lambda, R, P_\Lambda, P_R; N, N^r] \ , \end{aligned} \tag{2.8}$$

[2] Note that the super-Hamiltonian constraint implies $\Lambda_0^2 = 4R_0R_2$, from which it follows in particular that R_2 is positive on the classical solutions. The dynamical equation of motion for $\dot R$ implies $\dot R_0 = 0$.

where the boundary action is given by

$$S_{\partial\Sigma}[\Lambda, R, P_\Lambda, P_R; N, N^r] = \tfrac{1}{2}\int dt\,[R^2 N'\Lambda^{-1}]_{r=0} + \int dt\left[NRR'\Lambda^{-1} - N^r\Lambda P_\Lambda - \tfrac{1}{2}R\dot{R}\ln\left|\frac{N+\Lambda N^r}{N-\Lambda N^r}\right|\right]_{r=1} . \tag{2.9}$$

The variation of the total action (2.8) can be written as a sum of a volume term proportional to the equations of motion, boundary terms from the initial and final spatial surfaces, and boundary terms from $r = 0$ and $r = 1$. The boundary terms from the initial and final spatial surfaces take the usual form

$$\pm \int_0^1 dr\,(P_\Lambda \delta\Lambda + P_R \delta R) \ , \tag{2.10}$$

with the upper (lower) sign corresponding to the final (initial) surface. These terms vanish provided we fix the initial and final three-metrics. The boundary term from $r = 0$ takes, by virtue of the falloff conditions (2.6), the simple form

$$\tfrac{1}{2}\int dt\,[R^2\,\delta(N'\Lambda^{-1})]_{r=0} = \tfrac{1}{2}\int dt\,R_0^2\,\delta(N_1\Lambda_0^{-1}) \ , \tag{2.11}$$

which vanishes provided we fix the quantity $N_1\Lambda_0^{-1} = \lim_{r\to 0} N'\Lambda^{-1}$. In the classical solution this means, by Eq. (2.7), fixing the rate at which the unit normal to the constant t surface is boosted at the coordinate singularity at the bifurcation two-sphere. Finally, the boundary term from $r = 1$ reads

$$\int dt\left[[-P_R N^r + \Lambda^{-1}(NR)']\delta R - \tfrac{1}{2}\ln\left|\frac{N+\Lambda N^r}{N-\Lambda N^r}\right|\delta(R\dot{R}) + \tfrac{1}{2}N^{-1}R\left\{\Lambda N^r\dot{R}[N^2-(\Lambda N^r)^2]^{-1} + \Lambda^{-1}R'\right\}\right.$$
$$\left.\times\delta(N^2-(\Lambda N^r)^2) - [P_\Lambda + N^{-1}R(\dot{R}-R'N^r)]\delta(\Lambda N^r)\right]_{r=1} . \tag{2.12}$$

As R and $N^2 - (\Lambda N^r)^2$ are fixed at $r = 1$, the three first terms in (2.12) vanish. The integrand in the last term in (2.12) is proportional to the equation of motion (2.3a), which is classically enforced for $0 < r < 1$ by the volume term in the variation of the action. Therefore, for classical solutions, also the last term in (2.12) will vanish by continuity.

We thus conclude that the action (2.8) is appropriate for a variational principle which fixes the initial and final three-metrics, the three-metric on the timelike boundary at $r = 1$, and the quantity $N_1\Lambda_0^{-1} = \lim_{r\to 0} N'\Lambda^{-1}$. Each classical solution is part of the right hand exterior region of a Kruskal spacetime, with the constant t slices approaching the bifurcation two-sphere as $r \to 0$, and $N_1\Lambda_0^{-1}$ giving via (2.7) the rate of change of the unit normal to the constant t surfaces at the bifurcation two-sphere.

Although we are here using natural units, the argument of the cosh in (2.7) is a truly dimensionless "boost parameter" even in physical units. Having the quantity which is fixed at $r = 0$ be dimensionless will be important for arriving at our thermodynamical goal in Sec. V.

III. CANONICAL TRANSFORMATION

In this section we show that the canonical transformation given by Kuchař from the variables $\{\Lambda, P_\Lambda; R, P_R\}$ to the new variables $\{M, P_M; \mathsf{R}, P_{\mathsf{R}}\}$ is readily adapted to our boundary conditions. We shall from now on assume that the quantity R_2 in Eq. (2.6b) is positive; as noted in Sec. II, this is always the case for the classical solutions.

Recall from Kuchař that the new variables $\{M, P_M; \mathsf{R}, P_{\mathsf{R}}\}$ are defined by

$$M = \tfrac{1}{2}R(1-F) \ , \tag{3.1a}$$

$$P_M = R^{-1}F^{-1}\Lambda P_\Lambda \ , \tag{3.1b}$$

$$\mathsf{R} = R, \tag{3.1c}$$

$$P_{\mathsf{R}} = P_R - \tfrac{1}{2}R^{-1}\Lambda P_\Lambda - \tfrac{1}{2}R^{-1}F^{-1}\Lambda P_\Lambda - R^{-1}\Lambda^{-2}F^{-1}[(\Lambda P_\Lambda)'(RR') - (\Lambda P_\Lambda)(RR')'], \tag{3.1d}$$

where

$$F = \left(\frac{R'}{\Lambda}\right)^2 - \left(\frac{P_\Lambda}{R}\right)^2 . \tag{3.2}$$

In the classical solution, M is the value of the Schwarzschild mass and $-P_M$ is the derivative of the Killing time with respect to r. A pair of quantities which will become new Lagrange multipliers is defined by

$$\mathsf{N} = (4M)^{-1}\left(NF^{-1}\Lambda^{-1}R' - N^r R^{-1}F^{-1}\Lambda P_\Lambda\right), \tag{3.3a}$$

$$N^{\mathsf{R}} = N^r R' - NR^{-1}P_\Lambda \ . \tag{3.3b}$$

The falloff conditions (2.6) imply

$$M(t,r) = \tfrac{1}{2}\mathsf{R}_0(t) + M_2(t)r^2 + O(r^4) \ , \tag{3.4a}$$

$$\mathsf{R}(t,r) = \mathsf{R}_0(t) + \mathsf{R}_2(t)r^2 + O(r^4) \ , \tag{3.4b}$$

$$P_M(t,r) = O(r) \ , \tag{3.4c}$$

$$P_\mathsf{R}(t,r) = O(r) \ , \tag{3.4d}$$

$$\mathsf{N}(t,r) = \mathsf{N}_0(t) + O(r^2) \ , \tag{3.4e}$$

$$N^\mathsf{R}(t,r) = N_2^\mathsf{R}(t)r^2 + O(r^4) \ , \tag{3.4f}$$

where $\mathsf{R}_0 = R_0 > 0$, $\mathsf{R}_2 = R_2 > 0$, $M_2 = \frac{1}{2}R_2\left(1 - 4R_0R_2\Lambda^{-2}\right)$, $\mathsf{N}_0 = \frac{1}{4}N_1\Lambda_0R_0^{-1}R_2^{-1} \geq 0$, and $N_2^\mathsf{R} = 2N_1^r R_2$. We also have

$$F(t,r) = 4R_2^2\Lambda_0^{-2}r^2 + O(r^4) \ . \tag{3.5}$$

The transformation equations (3.1)–(3.3) are almost identical to those given by Kuchař. The only exception is that instead of our N [Eq. (3.3a)], Kuchař adopts the Lagrange multiplier N^M defined by

$$N^M = -4M\mathsf{N} \ . \tag{3.6}$$

Our reasons for choosing N will be discussed near the end of the section.

Demonstrating that the transformation (3.1) is a canonical transformation under our boundary conditions is analogous to the similar demonstration given by Kuchař for the asymptotically Kruskal case. We start from the identity

$$\begin{aligned} &P_\Lambda\delta\Lambda + P_R\delta R - P_M\delta M - P_\mathsf{R}\delta\mathsf{R} \\ &\quad = \left(\tfrac{1}{2}R\delta R\ln\left|\frac{RR' + \Lambda P_\Lambda}{RR' - \Lambda P_\Lambda}\right|\right)' \\ &\qquad + \delta\left(\Lambda P_\Lambda + \tfrac{1}{2}RR'\ln\left|\frac{RR' - \Lambda P_\Lambda}{RR' + \Lambda P_\Lambda}\right|\right) \ , \end{aligned} \tag{3.7}$$

and integrate both sides with respect to r from $r = 0$ to $r = 1$. On the right hand side, the first term is directly integrated and produces substitution terms from $r = 0$ and $r = 1$. The substitution term from $r = 0$ vanishes because the falloff conditions (3.4) make the logarithm vanish there, and the substitution term from $r = 1$ vanishes because δR vanishes there by our boundary conditions. We therefore obtain

$$\int_0^1 dr\,(P_\Lambda\delta\Lambda + P_R\delta R) - \int_0^1 dr\,(P_M\delta M + P_\mathsf{R}\delta\mathsf{R}) = \delta\omega\left[\Lambda, P_\Lambda, R\right], \tag{3.8}$$

where

$$\omega\left[\Lambda, P_\Lambda, R\right] = \int_0^1 dr\left(\Lambda P_\Lambda + \tfrac{1}{2}RR'\ln\left|\frac{RR' - \Lambda P_\Lambda}{RR' + \Lambda P_\Lambda}\right|\right). \tag{3.9}$$

Equations (3.8) and (3.9) show that the Liouville forms of the old and new variables differ only by an exact form. The transformation is therefore canonical. If desired, the generating functional of the transformation is easily read off from the corresponding functional given by Kuchař. Also, the transformation is easily invertible; the explicit expressions for the inverse transformation were given by Kuchař.

The canonical transformation (3.1) becomes singular when $F = 0$, and the Lagrange multiplier redefinition (3.3a) becomes singular when $F = 0$ or $M = 0$. Under our boundary conditions the classical solutions have always $M > 0$, and they also have $0 < F < 1$ for $r > 0$. At the limit $r \to 0$, F approaches zero according to (3.5), but (3.1) and (3.3) have the well-defined limits given in (3.4). Our canonical transformation is therefore well defined and differentiable near the classical solutions, and similarly the inverse transformation is well defined and differentiable near the classical solutions. From now on we shall assume that we are always in such a neighborhood of the classical solutions that $M > 0$ holds, and $0 < F < 1$ holds for $r > 0$.

We wish to write an action in terms of the new variables. Using Eqs. (3.3), one sees as in the paper by Kuchař that the constraint terms $NH + N^rH_r$ in the old surface action (2.4) take the form $-4\mathsf{N}MM' + N^\mathsf{R}P_\mathsf{R}$. We can therefore take the new surface action to be

$$S_\Sigma[M, \mathsf{R}, P_M, P_\mathsf{R}; \mathsf{N}, N^\mathsf{R}] = \int dt \int_0^1 dr\left(P_M\dot{M} + P_\mathsf{R}\dot{\mathsf{R}} + 4\mathsf{N}MM' - N^\mathsf{R}P_\mathsf{R}\right) \ , \tag{3.10}$$

where the quantities to be varied independently are M, R, P_M, P_R, N, and N^R. The full set of equations of motion reads

$$\dot{M} = 0 \ , \tag{3.11a}$$

$$\dot{\mathsf{R}} = N^\mathsf{R} \ , \tag{3.11b}$$

$$\dot{P}_M = -4M\mathsf{N}' \ , \tag{3.11c}$$

$$\dot{P}_\mathsf{R} = 0 \ , \tag{3.11d}$$

$$MM' = 0 \ , \tag{3.11e}$$

$$P_\mathsf{R} = 0 \ . \tag{3.11f}$$

We now turn to the boundary conditions and boundary terms. As a preparation for this, let us denote by Q^2 the quantity $-g_{tt}$ when expressed as a function of the new canonical variables and Lagrange multipliers. A short calculation using (3.1)–(3.3) yields

$$Q^2 = -g_{tt} = 16M^2\mathsf{F}\mathsf{N}^2 - \mathsf{F}^{-1}\left(N^\mathsf{R}\right)^2 \ , \tag{3.12}$$

where $\mathsf{F} = 1 - 2M\mathsf{R}^{-1}$. In general, Q^2 need not be positive for all values of r, even for classical solutions. However, as in Sec. II, we shall introduce boundary conditions that fix the intrinsic metric of the three-surface $r = 1$ to be timelike, and under such boundary conditions Q^2 is positive at $r = 1$. From (3.12) it is then seen that N is nonzero at $r = 1$. Recalling that we are assuming $N > 0$, Eq. (3.3a) shows that N is positive at $r = 1$ for classical solutions with the Schwarzschild slicing, since in this slicing one has $P_\Lambda = 0$. Continuity then implies that N must be positive at $r = 1$ for all classical solutions compatible with our boundary conditions. We can therefore, without loss of generality, choose to work in a neighborhood of the classical solutions such that N is positive at $r = 1$.

Consider now the total action

$$S[M, \mathsf{R}, P_M, P_{\mathsf{R}}; \mathsf{N}, N^{\mathsf{R}}] = S_\Sigma[M, \mathsf{R}, P_M, P_{\mathsf{R}}; \mathsf{N}, N^{\mathsf{R}}] + S_{\partial\Sigma}[M, \mathsf{R}, P_M, P_{\mathsf{R}}; \mathsf{N}, N^{\mathsf{R}}], \tag{3.13}$$

where the boundary action is given by

$$S_{\partial\Sigma}[M, \mathsf{R}, P_M, P_{\mathsf{R}}; \mathsf{N}, N^{\mathsf{R}}] = 2\int dt\, [M^2\mathsf{N}]_{r=0} + \int dt \left[\mathsf{R}\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} + \tfrac{1}{2}\mathsf{R}\dot{\mathsf{R}}\ln\left(\frac{\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} - \dot{\mathsf{R}}}{\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} + \dot{\mathsf{R}}}\right)\right]_{r=1} . \tag{3.14}$$

Note that the argument of the logarithm in (3.14) is always positive. The variation of (3.13) contains a volume term proportional to the equations of motion, as well as several boundary terms. From the initial and final spatial surfaces one gets the usual boundary terms

$$\pm \int_0^1 dr\, (P_M \delta M + P_{\mathsf{R}} \delta \mathsf{R}) \quad , \tag{3.15}$$

which vanish provided we fix M and R on these surfaces. The boundary term from $r = 0$ is

$$2\int dt [M^2\delta\mathsf{N}]_{r=0} = \tfrac{1}{2}\int dt\, \mathsf{R}_0^2 \delta\mathsf{N}_0 \quad , \tag{3.16}$$

which vanishes provided we fix N_0. In the classical solution, the time evolution of the unit normal to the spatial surfaces at $r \to 0$ will then be given by (2.7) with $\Lambda_0^{-1}(t)N_1(t) = \mathsf{N}_0(t)$. Finally, the boundary term from $r = 1$ is the integral over t of

$$A_{\mathsf{R}}\, \delta\mathsf{R} + A_{\dot{\mathsf{R}}}\, \delta\dot{\mathsf{R}} + A_{Q^2}\, \delta(Q^2) + \left[\frac{\left(N^{\mathsf{R}}\right)^2 - \dot{\mathsf{R}}^2}{\mathsf{F}\left(\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} + 4M\mathsf{F}\mathsf{N}\right)}\right] \delta M \quad , \tag{3.17}$$

where A_{R}, $A_{\dot{\mathsf{R}}}$, and A_{Q^2} are functions whose explicit form will not be important here. As before, we wish to fix the intrinsic metric on the timelike surface $r = 1$. From the above discussion this means fixing R and Q^2 to be prescribed positive functions of t at $r = 1$. The first three terms in (3.17) therefore vanish. The last term in (3.17) is proportional to the equation of motion (3.11b), which is classically enforced for $0 < r < 1$ by the volume term in the variation of the action. Therefore, for classical solutions, also the last term in (3.17) will vanish by continuity. Note that the assumption that N is positive is needed for ensuring that the denominator of the last term in (3.17) is nonvanishing when the equation of motion (3.11b) holds.

We have thus identified the quantities to be held fixed in the variational problem associated with the action (3.13). At the initial and final three-surfaces one fixes the new canonical coordinates M and R, at $r = 1$ one fixes the intrinsic metric on the timelike three-surface, and at $r = 0$ one fixes the quantity N_0 which in the classical solutions determines the time evolution of the unit normal to the spatial surfaces at the bifurcation two-sphere via (2.7) with $\Lambda_0^{-1}(t)N_1(t) = \mathsf{N}_0(t)$. At $r = 0$ and $r = 1$, these conditions are identical to those appropriate for the metric action (2.8).

It is instructive to consider what happens if one follows Kuchař and replaces the Lagrange multiplier N by N^M according to Eq. (3.6). Note first that the falloff condition for N^M at $r \to 0$ is

$$N^M(t, r) = N_0^M(t) + O(r^2) \quad , \tag{3.18}$$

where $N_0^M = -2\mathsf{R}_0\mathsf{N}_0 = -\frac{1}{2}N_1\Lambda_0 R_2^{-1} \leq 0$. An action corresponding to (3.13) can now be written as

$$\begin{aligned} S[M, \mathsf{R}, P_M, P_{\mathsf{R}}; N^M, N^{\mathsf{R}}] &= S_\Sigma[M, \mathsf{R}, P_M, P_{\mathsf{R}}; N^M, N^{\mathsf{R}}] \\ &\quad + S_{\partial\Sigma}[M, \mathsf{R}, P_M, P_{\mathsf{R}}; N^M, N^{\mathsf{R}}] \quad , \end{aligned} \tag{3.19}$$

where the surface action is given by

$$S_\Sigma[M, \mathsf{R}, P_M, P_{\mathsf{R}}; N^M, N^{\mathsf{R}}] = \int dt \int_0^1 dr \left(P_M \dot{M} + P_{\mathsf{R}} \dot{\mathsf{R}} - N^M M' - N^{\mathsf{R}} P_{\mathsf{R}}\right) \quad , \tag{3.20}$$

and the boundary action by

$$S_{\partial\Sigma}[M, \mathsf{R}, P_M, P_{\mathsf{R}}; N^M, N^{\mathsf{R}}] = -\int dt\, [MN^M]_{r=0} + \int dt \left[\mathsf{R}\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} + \tfrac{1}{2}\mathsf{R}\dot{\mathsf{R}}\ln\left(\frac{\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} - \dot{\mathsf{R}}}{\sqrt{\mathsf{F}Q^2 + \dot{\mathsf{R}}^2} + \dot{\mathsf{R}}}\right)\right]_{r=1} . \tag{3.21}$$

Here $\mathsf{F} = 1 - 2M\mathsf{R}^{-1}$ as before, and Q^2 is understood via (3.6) and (3.12) as a function of the variables appearing in the surface action (3.20). The quantities varied independently are M, R, P_M, P_{R}, N^M, and N^{R}. It can now be verified as above that the fixed quantities at the initial and final surfaces and at $r = 1$ are identical to those with the action (3.13). However, the boundary term in the variation of (3.19) at $r = 0$ is

$$-\int dt \left[M\delta N^M\right]_{r=0} = -\tfrac{1}{2}\int dt\, \mathsf{R}_0 \delta N_0^M \quad . \tag{3.22}$$

To make (3.22) vanish, one needs to fix N_0^M. In the classical solution, the time evolution of the unit normal to the spatial surfaces at $r \to 0$ will then be given by (2.7) with $\Lambda_0^{-1}(t)N_1(t) = -\frac{1}{4}M^{-1}N_0^M(t)$. While this is qualitatively similar to the boundary condition appropriate for the action (3.13), there is an important quantitative difference: The quantity N_0 fixed in the action (3.13) gives directly the time derivative of the boost parameter at the bifurcation two-sphere, but the quantity N_0^M fixed in the action (3.19) is proportional to the time derivative of the boost parameter by a coefficient that depends explicitly on the canonical variable M. This feature of the action (3.19) poses no difficulty at the classical level, or even in the construction of a quantum theory, but it will be seen later that this would present a problem in connecting the quantum theory to our thermodynamical goal. We shall therefore proceed using the action (3.13).

To end this section, we note that one could obtain new actions appropriate for the boundary conditions given above by replacing the boundary actions (3.14) and (3.21) by expressions that are equivalent when the classical equations of motion hold. As the volume terms in the variation of the actions enforce the classical equations of motion for $0 < r < 1$, continuity implies that such a replacement does not change the critical points of the action. For example, in (3.14) the term from $r = 1$ could be replaced by

$$\int dt \left[4M\mathsf{RFN} + \tfrac{1}{2}\mathsf{R}\dot{\mathsf{R}} \ln \left|\frac{4M\mathsf{FN} - \dot{\mathsf{R}}}{4M\mathsf{FN} + \dot{\mathsf{R}}}\right|\right]_{r=1} \quad . \tag{3.23}$$

Such replacements would clearly not affect the Hamiltonian reduction that we shall perform in the next section. Our reason for choosing (3.14) is merely that of simplicity: It is a function of the boundary data and the canonical variable M only. This will make the Hamiltonian reduction especially straightforward.

IV. HAMILTONIAN REDUCTION

We now concentrate on the variational principle associated with the action $S[M, \mathsf{R}, P_M, P_{\mathsf{R}}; \mathsf{N}, N^{\mathsf{R}}]$ [Eq. (3.13)]. We shall reduce the action to the true dynamical degrees of freedom by solving the constraints.

The constraint $MM' = 0$ [Eq. (3.11e)] implies that M is independent of r. We can therefore write

$$M(t, r) = \mathbf{m}(t) \quad . \tag{4.1}$$

Substituting this and the constraint $P_{\mathsf{R}} = 0$ (3.11f) back into (3.13) yields the true Hamiltonian action

$$S[\mathbf{m}, \mathbf{p}; \mathsf{N}_0; \mathsf{R}_B, Q_B] = \int dt\, (\mathbf{p}\dot{\mathbf{m}} - \mathbf{h}) \quad , \tag{4.2}$$

where

$$\mathbf{p} = \int_0^1 dr\, P_M \quad . \tag{4.3}$$

The reduced Hamiltonian $\mathbf{h}$ in (4.2) takes the form

$$\mathbf{h} = \mathbf{h}_H + \mathbf{h}_B \quad , \tag{4.4}$$

with

$$\mathbf{h}_H = -2\mathsf{N}_0\mathbf{m}^2 \quad , \tag{4.5a}$$

$$\mathbf{h}_B = -\mathsf{R}_B\sqrt{\mathsf{F}_B Q_B^2 + \dot{\mathsf{R}}_B^2} - \tfrac{1}{2}\mathsf{R}_B\dot{\mathsf{R}}_B \ln\left(\frac{\sqrt{\mathsf{F}_B Q_B^2 + \dot{\mathsf{R}}_B^2} - \dot{\mathsf{R}}_B}{\sqrt{\mathsf{F}_B Q_B^2 + \dot{\mathsf{R}}_B^2} + \dot{\mathsf{R}}_B}\right) \quad . \tag{4.5b}$$

Here R_B and Q_B^2 are the values of R and Q^2 at the timelike boundary $r = 1$, and $\mathsf{F}_B = 1 - 2\mathbf{m}\mathsf{R}_B^{-1}$. R_B, Q_B^2, and N_0 are considered to be prescribed functions of time, satisfying $\mathsf{R}_B > 0$, $Q_B^2 > 0$, and $\mathsf{N}_0 \geq 0$. Note that $\mathbf{h}$ is, in general, explicitly time dependent.

The variational principle associated with the reduced action (4.2) fixes the initial and final values of $\mathbf{m}$. The equations of motion are

$$\dot{\mathbf{m}} = 0 \quad , \tag{4.6a}$$

$$\dot{\mathbf{p}} = -\frac{\partial \mathbf{h}}{\partial \mathbf{m}} = 4\mathbf{m}\mathsf{N}_0 - \mathsf{F}_B^{-1}\sqrt{\mathsf{F}_B Q_B^2 + \dot{\mathsf{R}}_B^2} \quad . \tag{4.6b}$$

Equation (4.6a) is readily understood in terms of the statement that $\mathbf{m}$ is classically equal to the time-independent value of the Schwarzschild mass. To interpret equation (4.6b), recall from Kuchař and Sec. III that $-P_M$ equals classically the derivative of the Killing time with respect to r, and $\mathbf{p}$ therefore equals, by (4.3), the difference of the Killing times at the left and right ends of the constant t surface. As the constant t surface evolves in the Schwarzschild spacetime, the first term in (4.6b) gives the evolution rate of the Killing time at the left end of the surface, where the surface terminates at the bifurcation two-sphere, and the second term in (4.6b) gives the negative of the evolution rate of the Killing time at the right end of the surface, where the surface terminates at the timelike boundary. The two terms are clearly generated respectively by $\mathbf{h}_H$ [Eq. (4.5a)] and $\mathbf{h}_B$ [Eq. (4.5b)].

The case of most physical interest in the quantum theory is when the radius of the boundary two-sphere does not change in time, $\dot{\mathsf{R}}_B = 0$. The second term in $\mathbf{h}_B$ (4.5b) then vanishes, and the second term in (4.6b) is readily understood in terms of the Killing time of a static Schwarzschild observer, expressed as a function of the proper time $\int^t dt' \sqrt{Q_B^2(t')}$ and the blueshift factor $\mathsf{F}_B^{-1/2}$. We shall concentrate on this case in the quantum theory in the next section.

V. QUANTUM THEORY AND THE PARTITION FUNCTION

We now proceed to quantize the reduced Hamiltonian theory of Sec. IV in the special case $\dot{\mathsf{R}}_B = 0$. As explained in the Introduction, our aim is to construct the time evolution operator in a Hamiltonian quantum theory, and then to obtain a partition function via an analytic continuation of this operator.

A. Quantization

Let us first rewrite the classical theory in a more convenient notation. We take the action to be

$$S[\mathbf{m}, \mathbf{p}; \mathsf{N}_0, Q_B; B] = \int dt\, (\mathbf{p}\dot{\mathbf{m}} - \mathbf{h}) \quad , \tag{5.1}$$

where the Hamiltonian $\mathbf{h}$ is given by

$$\mathbf{h} = \left(1 - \sqrt{1 - 2\mathbf{m}B^{-1}}\right) B Q_B - 2\mathsf{N}_0 \mathbf{m}^2 \quad . \tag{5.2}$$

Here $\mathsf{N}_0 \geq 0$ and $Q_B = \sqrt{Q_B^2} > 0$ are prescribed functions of the time t, as defined in the previous sections, and $B > 0$ is the time-independent value of R_B. Compared with Sec. IV, we have added to the Hamiltonian the term BQ_B. As this term is independent of the canonical variables, it does not affect the equations of motion. It is equal to the K_0 term of Gibbons and Hawking [1], evaluated at the timelike boundary, and its purpose here is to renormalize the energy in the fashion discussed in Ref. [15]. The canonical momentum $\mathbf{p}$ takes all real values, whereas the canonical coordinate $\mathbf{m}$ is restricted to lie in the range $0 < \mathbf{m} < \frac{1}{2}B$.

As is well known, the quantization of a given classical Hamiltonian theory requires additional input [39–41]. In our case, one would in particular expect complications from the global properties of the classical theory: One cannot promote $\mathbf{m}$ and $\mathbf{p}$ to self-adjoint operators $\hat{\mathbf{m}}$ and $\hat{\mathbf{p}}$ with the commutator $[\hat{\mathbf{m}}, \hat{\mathbf{p}}] = i$ such that the spectrum of $\hat{\mathbf{m}}$ would coincide with the classical range of $\mathbf{m}$ [42]. It might be feasible to explore the possible quantum theories in the fashion discussed in Refs. [40,41], by starting from suitable Poisson bracket algebras of functions on the phase space of the reduced theory (5.1) and then promoting these algebras into quantum operator algebras; appropriate algebras could perhaps be obtained by considering functions related to specific classes of spacelike surfaces in the four-dimensional spacetime. However, as explained in the Introduction, our aim is to compare a partition function obtained from the Hamiltonian quantum theory to the semiclassical estimate obtained from the path integral approach. For such a semiclassical comparison, one may reasonably hope that the details of the Hamiltonian theory will not be crucial. We shall therefore follow a simpler path and define the quantum theory by fiat, but still in a mathematically precise way. While we shall not attempt to construct a complete set of operators in the Hilbert space by starting from some prescribed algebra of functions on the classical phase space, in the sense of Refs. [40,41], we shall define a quantum Hamiltonian operator that corresponds to the classical Hamiltonian $\mathbf{h}$ [Eq. (5.2)]. The full quantum operator algebra can be chosen to be, for example, the algebra of all bounded operators on the Hilbert space or any sufficiently large subalgebra thereof.

From now on, B will be considered fixed. We take the wave functions to be functions of the configuration variable $\mathbf{m}$, and the inner product is taken to be

$$(\psi, \chi) = \int_0^{B/2} d\mathbf{m}\, \overline{\psi(\mathbf{m})} \chi(\mathbf{m}) \quad . \tag{5.3}$$

The Hilbert space is thus $H = L_2([0, B/2])$. It would be straightforward to generalize this to an inner product where the integral in (5.3) includes a smooth positive weight function $\mu(\mathbf{m}; B)$: By writing $\widetilde{\mathbf{m}} = \int_0^{\mathbf{m}} d\mathbf{m}'\, \mu(\mathbf{m}'; B)$, such an inner product reduces to that in (5.3) with $\mathbf{m}$ replaced by $\widetilde{\mathbf{m}}$. For sufficiently slowly varying $\mu(\mathbf{m}; B)$, this generalization would not affect the thermodynamical results below. For simplicity, we shall adhere to (5.3).

The Hamiltonian operator $\hat{\mathbf{h}}(t)$ in H is taken to act as pointwise multiplication by the function $\mathbf{h}(\mathbf{m}; t)$ [Eq. (5.2)]. $\hat{\mathbf{h}}(t)$ is clearly bounded and self-adjoint. It depends explicitly on t through Q_B and N_0, but it commutes with itself at different values of t. The unitary time evolution operator in H is therefore given by

$$\hat{K}(t_2; t_1) = \exp\left[-i \int_{t_1}^{t_2} dt'\, \hat{\mathbf{h}}(t')\right] \quad . \tag{5.4}$$

From Eq. (5.2) one sees that $\hat{K}(t_2; t_1)$ acts in H as pointwise multiplication by the function

$$K(\mathbf{m}; T_B; \Theta_H) = \exp\left[-i\left(1 - \sqrt{1 - 2\mathbf{m}B^{-1}}\right) BT_B + 2i\mathbf{m}^2 \Theta_H\right] \quad , \tag{5.5}$$

where

$$T_B = \int_{t_1}^{t_2} dt\, Q_B(t) \quad , \tag{5.6a}$$

$$\Theta_H = \int_{t_1}^{t_2} dt\, \mathsf{N}_0(t) \quad . \tag{5.6b}$$

$\hat{K}(t_2; t_1)$ therefore depends on t_1 and t_2 only through the quantities T_B and Θ_H [Eq. (5.6)], and we can write it as $\hat{K}(T_B, \Theta_H)$. The composition law

$$\hat{K}(t_3; t_2)\hat{K}(t_2; t_1) = \hat{K}(t_3; t_1) \tag{5.7}$$

takes the form

$$\hat{K}(T_B, \Theta_H)\, \hat{K}(\tilde{T}_B, \tilde{\Theta}_H) = \hat{K}(T_B + \tilde{T}_B, \Theta_H + \tilde{\Theta}_H) \quad . \tag{5.8}$$

This means that the time evolution operator contains T_B and Θ_H as two independent evolution parameters. From (5.6) one sees that T_B can be interpreted as the proper time elapsed at the timelike boundary and Θ_H can be interpreted as the boost parameter elapsed at the bifurcation two-sphere.

B. Partition function

Having defined the time evolution operator $\hat{K}(T_B, \Theta_H)$, we now wish to continue this operator to imaginary time and to construct a partition function by taking the trace.

The envisaged thermodynamical situation consists of a Schwarzschild black hole at the center of a mechanically rigid spherical box, with the temperature at the box held fixed [15]. The thermodynamics is thus described by the canonical ensemble [14]. In the Euclidean path integral approach to computing the partition function, one identifies the inverse temperature at the box as the proper circumference in the periodic imaginary time direction. When the four-manifold in the path integral is chosen to be $\bar{D}^2 \times S^2$, which admits Euclidean Schwarzschild solutions, the saddle points of the path integral are either real Euclidean or complex Schwarzschild metrics, depending on the boundary data [15,16,43]. Under certain assumptions as to which of the saddle points dominate the integral, it can be shown that the resulting partition function is that of a thermodynamically stable ensemble. In the classically dominant domain, such a stable situation corresponds to the black hole being so large that the box is well within the closed photon orbit, and the thermodynamical stability is readily understood as a balance effect between the $(8\pi M)^{-1}$ behavior of the Hawking temperature as measured at the infinity and the $(1 - 2M/B)^{-1/2}$ blueshift factor between the infinity and the finite box radius. For details, see Refs. [15,16,21,28–31,43].

We now wish to relate this Euclidean path integral description to our Lorentzian Hamiltonian theory. In particular, we wish to set the evolution parameters of the time evolution operator $\hat{K}(T_B, \Theta_H)$ to values that, upon taking the trace, would yield a partition function in agreement with the semiclassical estimate to the Euclidean path integral.

Recall that T_B is the Lorentzian proper time elapsed at the timelike boundary. We therefore set $T_B = -i\beta$, and interpret β as the inverse temperature at the boundary. The case with Θ_H is less obvious, as no quantity corresponding to Θ_H directly appears in the setting of the Euclidean boundary value problem. However, what did appear in the Euclidean boundary value problem was the choice of the four-manifold, motivated by the existence of the desired classical Euclidean solutions. We follow the same logic here: We wish to choose Θ_H so that the classical solutions of the reduced Hamiltonian theory become solutions to the above Euclidean boundary value problem.

Now, the real Euclidean Schwarzschild solutions satisfy $\Theta_H = -2\pi i$. For the complex Schwarzschild solutions the freedom of performing complex diffeomorphisms gives rise to some arbitrariness [44], but one can consistently take the viewpoint that $\Theta_H = -2\pi i$ holds also for these complex-valued Schwarzschild solutions. In essence, $\Theta_H = -2\pi i$ is a regularity condition, eliminating the possibility of a conical singularity at the horizon of the Euclidean or complex Schwarzschild metric. We shall therefore set $\Theta_H = -2\pi i$.

We have thus arrived at being able to propose for the partition function the expression

$$Z(\beta) = \mathrm{Tr}\left[\hat{K}(-i\beta; -2\pi i)\right] \quad . \tag{5.9}$$

As it stands, (5.9) is divergent. Taking the trace formally in the δ-function normalized eigenstates $|\mathbf{m}\rangle$ of the multiplication operator $\hat{\mathbf{m}}$ yields

$$\begin{aligned} Z(\beta) &= \int_0^{B/2} d\mathbf{m}\, \langle \mathbf{m}|\hat{K}(-i\beta, -2\pi i)|\mathbf{m}\rangle \\ &= \int_0^{B/2} d\mathbf{m}\, K(\mathbf{m}; -i\beta; -2\pi i)\langle \mathbf{m}|\mathbf{m}\rangle \\ &= \delta(0) \int_0^{B/2} d\mathbf{m}\, K(\mathbf{m}; -i\beta; -2\pi i) \quad , \end{aligned} \tag{5.10}$$

which diverges by virtue of the infinite factor $\delta(0)$. The expression (5.10) suggests that the trace could be renormalized by replacing $\delta(0)$ by the finite "inverse volume" factor $2/B$. This would give the renormalized partition function

$$\begin{aligned} Z_{\mathrm{ren}}(\beta) = \frac{2}{B} \int_0^{B/2} d\mathbf{m}\, \exp\Big[- \Big(1 - \sqrt{1 - 2\mathbf{m}B^{-1}}\Big) B\beta \\ + 4\pi \mathbf{m}^2 \Big], \end{aligned} \tag{5.11}$$

where we have substituted the explicit expression (5.5) for $K(\mathbf{m}; -i\beta; -2\pi i)$. While the above manipulations are formal, in Appendix A we shall present a rigorous regularization of the trace and show that, upon eliminating the regulator after a renormalization by a multiplicative constant, the finite remainder is precisely (5.11). We therefore feel justified to adopt (5.11) as the definition of the renormalized partition function $Z_{\mathrm{ren}}(\beta)$.

It is now immediately seen that $Z_{\mathrm{ren}}(\beta)$ [Eq. (5.11)] is in semiclassical agreement with the expression derived in Ref. [28] for the partition function from the Euclidean path integral. Further, the agreement would be exact if we had included a suitable measure factor $\mu(\mathbf{m}; B)$ in the inner product (5.3). This means that our $Z_{\mathrm{ren}}(\beta)$ has the thermodynamical properties discussed in Ref. [28]. In particular, the canonical ensemble is thermodynamically stable for all values of β and B, and in the semiclassical domain ($B \gg 1$, $\beta/B < 32\pi/27$), $Z_{\mathrm{ren}}(\beta)$ can be approximated by the contribution from the thermodynamically stable saddle point. This is our main result.

VI. CONCLUSIONS AND DISCUSSION

In this paper we have addressed the classical and quantum Hamiltonian dynamics of a Schwarzschild black hole with boundary conditions that place the hole at the center of a finite spherical "box." In the classical Hamiltonian analysis, we chose the spatial slices of the 3+1 decomposed metric to embed in the Kruskal spacetime so that their left end is at the bifurcation two-sphere and the right end on a timelike three-surface in the right-hand-side exterior region. We then performed a Hamiltonian reduction of this system, adapting to our boundary conditions the method given by Kuchař in the case of the full Kruskal spacetime. We found that, as in the full Kruskal case, our system has a canonical pair of true degrees of freedom. One member of the pair is the Schwarzschild mass, and its conjugate momentum is related to the boundary conditions at the two ends of the spatial slices. We exhibited a reduced Hamiltonian formulation in which the true Hamiltonian has two independent terms, one corresponding to how the normal to the spatial surfaces is chosen to evolve at the coordinate singularity at the bifurcation two-sphere and the other corresponding to how the metric on the timelike boundary is chosen. Upon quantization, in the special case where the radius of the "box" is time independent, this led to a theory where the time evolution operator contains two independent evolution parameters, one related to the bifurcation two-sphere and the other to the timelike boundary.

A thermodynamical partition function was obtained by continuing the arguments of the time evolution operator to imaginary values and taking the trace. Choosing the argument at the bifurcation two-sphere in a way motivated by the classical Euclidean boundary value problem, and giving a renormalization of the formally divergent trace, we arrived at a partition function which is in agreement with the one previously obtained by Whiting and York [28] via a Hamiltonian reduction of the Euclidean path integral. Our partition function thus reproduces the thermodynamical predictions obtained in Ref. [28]. In particular, the heat capacity is positive for all values of the temperature, and the canonical ensemble is thus thermodynamically stable.

In the Hamiltonian variational problem set up in Sec. II, the boundary conditions adopted at the two ends of the spatial slices were in essence independent of each other. It would therefore be straightforward to formulate new variational problems where the "timelike boundary" condition or the "bifurcation two-sphere" condition of Sec. II is combined to the "asymptotic infinity" condition of Kuchař. For example, one could choose the slices to begin at the bifurcation two-sphere and reach to the right-hand-side asymptotic infinity. Also, one could choose "parallelogram"-type boundary conditions where one fixes the intrinsic metric of a timelike three-surface at both ends of the spatial slices. One could then investigate how to apply the canonical transformation (3.1) in each case. Although we shall not attempt to discuss this in detail here, it would appear that the conclusion of one canonical pair of true degrees of freedom is robust under changes in the boundary conditions; for further discussion, see Refs. [33–35]. It is only the geometrical interpretation of the momentum conjugate to the Schwarzschild mass that depends on the boundary conditions. In Appendixes B and C we shall show that a similar conclusion about a canonical pair of true degrees of freedom is obtained also when the Kruskal boundary conditions of Kuchař are replaced by conditions that enforce every classical solution to be the $\mathbb{R}P^3$ geon [37], which is a maximal non-Kruskal extension of the Schwarzschild spacetime with spatial topology $\mathbb{R}P^3 \setminus \{p\}$ and only one asymptotically flat region.

In the ADM variational principle of Sec. II, the term at the bifurcation two-sphere in the boundary action (2.9) is not conceptually new: Similar terms have appeared in the black hole context perhaps most explicitly in Refs. [9,23], and in the more limited context of Euclidean or complex minisuperspace analyses for example in Refs. [43,45]. What may be more surprising is the appearance of a logarithm in the term at the timelike boundary in (2.9). To understand this, let us for simplicity consider "parallelogram"-type boundary conditions, where one fixes the intrinsic metric on a timelike three-surface both at $r = 0$ and $r = 1$. From Sec. II it is seen that a Lagrangian action appropriate for these boundary conditions is given by

$$S[R,\Lambda;N,N^r] = S_\Sigma[R,\Lambda;N,N^r] + \int dt \left[NRR'\Lambda^{-1} - \tfrac{1}{2}R\dot{R}\ln\left|\frac{N+\Lambda N^r}{N-\Lambda N^r}\right| \right]\Bigg|_{r=0}^{r=1} , \tag{6.1}$$

where we have used the notation $A\big|_{r=0}^{r=1} = A(r=1) - A(r=0)$. It can now be verified that (6.1) is equal to

$$\begin{aligned}(16\pi)^{-1} &\int_{\mathcal{M}} d^4x\,\sqrt{-g}\,{}^{(4)}\mathbf{R} \\ &+(8\pi)^{-1}\int_{\partial_t\mathcal{M}} d^3x\,\sqrt{\gamma}\,K \;+\; (8\pi)^{-1}\int_{\partial_r\mathcal{M}} d^3x\,\sqrt{-\gamma}\,\Theta \\ &-(8\pi)^{-1}\int_{\partial_{tr}\mathcal{M}} d^2x\,\sqrt{\gamma}\,\mathrm{arcsinh}(u^a n_a)\ ,\end{aligned} \tag{6.2}$$

evaluated for our spherically symmetric metric (2.1). Here $\mathcal{M} \simeq I\times I\times S^2$ is the spacetime manifold, $\partial_t\mathcal{M}$ is its spacelike boundary consisting of the initial and final components $I \times S^2$, $\partial_r\mathcal{M}$ is similarly its timelike boundary consisting of the left and right components $I \times S^2$, and $\partial_{tr}\mathcal{M}$ consists of the four corners, each homeomorphic to S^2. $\sqrt{-g}\,{}^{(4)}\mathbf{R}$ is the four-dimensional Ricci scalar density, K and Θ are, respectively, the traces of the extrinsic curvature tensors on $\partial_t\mathcal{M}$ and $\partial_r\mathcal{M}$, and γ stands for the determinant of the relevant (three- or two-dimensional) induced metric. u^a and n^a are, respectively, the outward unit normals to $\partial_t \mathcal{M}$ and $\partial_r \mathcal{M}$. The conventions are those of Ref. [46]. The logarithm in the boundary terms in (6.1) arises by noting that

$$\operatorname{arcsinh}(u^a n_a) = \pm \tfrac{1}{2} \ln \left| \frac{N + \Lambda N^r}{N - \Lambda N^r} \right| \quad , \tag{6.3}$$

where the sign is positive for the upper right and lower left corners and negative for the other two corners, and integrating certain terms in (6.2) by parts. The expression (6.2) gives, for metrics not necessarily sharing our symmetry assumptions, an action principle appropriate for fixing the intrinsic metric on all the smooth components of the boundary [47,48].

In the presence of timelike boundaries, it has been suggested [10] that another variational principle of interest is obtained by fixing, in addition to the three-metric on all the smooth components of the boundary, also the product $u^a n_a$ at the corners where the spacelike and timelike boundaries meet. The appropriate Lagrangian action is obtained by dropping the last term in (6.2). It appears not to be clear what the pertinent criteria would be for discussing the relative advantages of these two variational principles. One might perhaps hope to investigate this issue by analyzing the classical boundary value problem: One would expect to fix in the variational principle a set of boundary data under which the classical boundary value problem has a unique solution.[3] This criterion has however two problems. First, the hyperbolic nature of the Einstein equations makes it unclear what one would want to accept as independent boundary data in the classical boundary value problem in the presence of timelike boundaries. Second, for quantum mechanical purposes, the existence of solutions to the classical boundary value problem need not always be a relevant criterion.[4]

We have assumed throughout the paper that the spacetime metric is nondegenerate, with the exception of the carefully controlled coordinate singularity at the bifurcation two-sphere. If desired, this assumption would be easy to relax. For example, in the Hamiltonian metric action (2.8) it is possible, and arguably even natural, to allow the lapse N to take negative values [50–52]. In the action (3.13) and the reduced Hamiltonian theory of Sec. IV most of the explicit reference to the spacetime metric has disappeared, and the quantum theory of Sec. V is therefore not sensitive to the precise degree of degeneracy of the metric.

Throughout Secs. II–IV, we chose the classical variational principles in anticipation of the thermodynamical boundary conditions that were finally adopted in Sec. V. In particular, in Sec. III we chose to replace the Lagrange multiplier N^M adopted by Kuchař by the multiplier N which is related to N^M through the rescaling (3.6). This resulted in making the fixed quantity at the bifurcation two-sphere directly the time derivative of the boost parameter, rather than this derivative multiplied by a function of one of the canonical variables. Without the rescaling, we could still have gone through the Hamiltonian reduction of Sec. IV and constructed a quantum theory along the lines of Sec. V A. The time evolution operator of the quantum theory would again have contained two evolution parameters: the proper time T_B at the timelike boundary as before and a new parameter $\bar{\Theta}_H$ at the bifurcation two-sphere. However, it is quite difficult to see what could have been done to $\bar{\Theta}_H$ to obtain a partition function with the desired properties. The problem is that when the regularity condition at the Euclidean horizon is expressed in terms of $\bar{\Theta}_H$, it involves explicitly the Schwarzschild mass $\mathbf{m}$. As taking the trace of the time evolution operator contains an integration over $\mathbf{m}$, it is not possible to fix $\bar{\Theta}_H$ in the partition function to some numerical constant such that the classical solutions to the reduced Hamiltonian theory with this boundary data would become the Euclidean (or complex) Schwarzschild metrics.

At the end of Sec. III we pointed out that one can use the classical equations of motion to change the functional form of the boundary action in the unreduced classical theory without affecting the boundary data, the critical points of the action, or the Hamiltonian reduction process of Sec. IV. While this observation is rather trivial, there is a subtly less trivial way of changing the boundary terms so that neither the boundary data nor the critical points change, but the class of configurations within which the action is varied changes. To see this, consider the metric variables of Sec. II, and replace in the boundary action (2.9) the term at $r = 0$ by

$$\tfrac{1}{2} \int dt\, \tilde{\mathsf{N}}_0 R_0^2 \quad , \tag{6.4}$$

where $\tilde{\mathsf{N}}_0(t)$ is a prescribed function. The boundary data in the resulting variational principle then differ from the boundary data for (2.8) only in that the quantity $N_1 \Lambda_0^{-1} = \lim_{r\to 0} N' \Lambda^{-1}$ can now be freely varied; however, the variation with respect to R yields the new equa-

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[3] Perhaps one example deserves to be mentioned in this context. Consider the spherically symmetric geometries (2.1). Choose the initial and final surfaces to be flat [49], and choose the left and right timelike surfaces to be at constant values of the radius of the two-sphere. Consider now giving as the boundary data the values of the radius of the two-sphere on the right and left timelike boundaries, and the proper times elapsed at these two timelike boundaries. Embedding the resulting parallelogram into a Schwarzschild spacetime shows that the boundary value problem has at most a discrete set of solutions. In each member of this discrete set the Schwarzschild mass is uniquely determined, and so are the values of $u^a n_a$ at the four corners. One is therefore not free to specify generic values for $u^a n_a$ at the corners as additional boundary data.

[4] As an example, consider the free nonrelativistic particle in the momentum representation. The path integral giving the time evolution operator fixes the initial and final momenta, but the classical boundary value problem with this boundary data has generically no solution. We thank David Brown for emphasizing this example to us.

tion of motion $N_1\Lambda_0^{-1} = \tilde{\mathsf{N}}_0$. Thus, the classical solutions have the same boundary data as before. Similarly, in the new canonical variables of Sec. III one obtains the analogous variational principle by replacing in the boundary action (3.14) the term at $r = 0$ by

$$2\int dt\, \tilde{\mathsf{N}}_0 \left[M^2\right]_{r=0} \quad , \tag{6.5}$$

where $\tilde{\mathsf{N}}_0(t)$ is prescribed function as above. N_0 can now be freely varied, but the variation with respect to M yields the equation of motion $\mathsf{N}_0 = \tilde{\mathsf{N}}_0$: Again, the boundary data for the classical solutions have not changed. When one carries out the Hamiltonian reduction of Sec. IV for the action with the boundary term (6.5), the only change is that N_0 in the Hamiltonian $\mathbf{h}_H$ [Eq. (4.5a)] gets replaced by $\tilde{\mathsf{N}}_0$. In terms of the geometrical boundary data, the reduced theory has therefore not changed at all. The quantization and the construction of the partition function can therefore be performed exactly as before.

The interest in the boundary terms (6.4) and (6.5) is that they are analogous to terms that appear naturally in the Euclidean actions that allow conical singularities at the Euclidean horizon [12,30,53–55]: Our Lorentzian boost parameter is analogous to the Euclidean deficit angle. In the Euclidean variational principle based on such an action, the variation with respect to the horizon area yields the vanishing of the deficit angle as an equation of motion. Both the horizon area and the deficit angle can therefore be regarded as "degrees of freedom" that contribute to path integrals, and it has been suggested that black hole entropy could be understood in terms of these horizon degrees of freedom [54,55]. Related viewpoints have been recently explored in Refs. [56,57]. From the Hamiltonian viewpoint of the present paper, it does not seem to make a difference whether one starts from an action in which the boost parameter is specified as a direct boundary condition or only indirectly as a consequence of an equation of motion. In both cases the elimination of the Hamiltonian constraints leads to the same reduced Hamiltonian theory.

We saw in Sec. V that the partition function $Z_{\text{ren}}(\beta)$ [Eq. (5.11)], at which we arrived by canonically quantizing the reduced Hamiltonian theory, is in semiclassical agreement with the partition function derived in Ref. [28] from a Euclidean path integral. Further, the agreement could have been made exact by including a suitable weight function $\mu(\mathbf{m}; B)$ in the inner product (5.3). With hindsight, this agreement should not be surprising. The path integral construction of Ref. [28] (see also Refs. [21,29]) is based on a classical elimination of the Hamiltonian constraint in a minisuperspace-type path integral with boundary conditions appropriate for a Euclidean black hole. What remains after the classical reduction is an ordinary integral over a single quantity, related to the area of the Euclidean horizon, and the only truly quantum mechanical input is the choice of the measure for this ordinary integration. In our Hamiltonian theory, we have similarly performed first a classical reduction by eliminating the Hamiltonian constraints, and the resulting configuration variable $\mathbf{m}$ is classically related to the area of the horizon. The continuation of the time evolution operator to imaginary time was fixed by a comparison with Euclidean black hole geometries, and the only truly quantum mechanical input in taking the trace of the time evolution operator was the choice of the Hilbert space of the quantum theory. It is quite natural that for inner products that are obtained by generalizing (5.3) by a weight factor $\mu(\mathbf{m}; B)$, the weight factor is in a direct correspondence with the choice of the path measure in Ref. [28].

It is perhaps appropriate to recall some thermodynamical properties of the partition function $Z_{\text{ren}}(\beta)$ [Eq. (5.11)]. Thermodynamical stability for all values of β and B has already been mentioned. In the semiclassical domain the integral in (5.11) is dominated by a classical Euclidean black hole solution, and the entropy, $S = [1 - \beta(\partial/\partial\beta)](\ln Z_{\text{ren}})$, to leading order, takes the Bekenstein-Hawking value; for details, see Ref. [28]. Further, in the semiclassical domain, the energy E and surface pressure P that are thermodynamically conjugate to β and $A = 4\pi B^2$,

$$E = -\frac{\partial\,(\ln Z_{\text{ren}})}{\partial\beta} \quad , \tag{6.6a}$$

$$P = \beta^{-1}\frac{\partial\,(\ln Z_{\text{ren}})}{\partial A} \quad , \tag{6.6b}$$

are, to leading order, the quantities that obey additivity laws for a shell with surface area A in equilibrium around a black hole [7,15,58,59]. However, the limit $B \to \infty$ with fixed β does not exist. This reflects the well-known instability of the canonical ensemble for a Schwarzschild hole in asymptotically flat space [7].

Comparing our derivation of the expression (5.11) for $Z_{\text{ren}}(\beta)$ to the Euclidean path integral derivation of the similar expression in Ref. [28], it is seen that the term in the exponent of (5.11) that arose from the bifurcation two-sphere contribution to the Lorentzian Hamiltonian is precisely the so-called entropy term in the Euclidean action. In light of this, it might be interesting to assess the similarities between our treatment of the bifurcation two-sphere and the Lorentzian Noether charge construction of the black hole entropy in Refs. [60,61].

It may be possible to define different Lorentzian Hamiltonian quantum theories with our boundary conditions by working in different canonical variables, and possibly without eliminating the constraints prior to the quantization. Although one would expect the partition functions obtained from such theories to be in semiclassical agreement with our $Z_{\text{ren}}(\beta)$ [Eq. (5.11)], there may nevertheless be qualitative differences in some thermodynamical quantities of interest. Examples of such differences are provided by the partition functions that were obtained from Euclidean path integral constructions in Refs. [30,31]. These partition functions agree semiclassically with our $Z_{\text{ren}}(\beta)$ [Eq. (5.11)], but they produce, in the terminology of Refs. [16,28–31], a qualitatively different energy spectrum.

In Sec. V, we included in the Hamiltonian $\mathbf{h}$ [Eq. (5.2)] the term BQ_B, which corresponds to the K_0 term of Gibbons and Hawking [1]. In the partition function, the role of this term is to renormalize the energy in the fashion discussed in Ref. [15]. By virtue of this term, $\mathbf{h}$ has at $B \to \infty$ the well-defined limit

$$\mathbf{h}_\infty = \mathbf{m}Q_\infty - 2\mathsf{N}_0\mathbf{m}^2 \quad , \tag{6.7}$$

where Q_∞ gives the proper time elapsed at the spatial infinity. It is clear that the classical theory with $\mathbf{h}_\infty$ can be quantized along the lines of Sec. V A, with the Hilbert space being $L_2([0,\infty))$. However, for the partition function one now recovers the formal expression

$$Z_\infty(\beta) = \delta(0) \int_0^\infty d\mathbf{m} \exp\left(-\mathbf{m}\beta + 4\pi\mathbf{m}^2\right) \quad , \tag{6.8}$$

which remains divergent even after dropping the infinite factor $\delta(0)$. This divergence is related to the above-mentioned nonexistence of the limit $B \to \infty$ in $Z_{\rm ren}(\beta)$ [Eq. (5.11)], and it can be regarded as the cause of the instability of the canonical ensemble for a Schwarzschild hole in asymptotically flat space.

Given the connections of the present work to Euclidean variational principles, one is prompted to ask whether it would be possible to adapt our classical variational analysis and Hamiltonian reduction to the Euclidean black hole. The analogue of the transformation (3.1), (3.2) in the Euclidean signature is easily found; the only difference is that (3.2) gets replaced by

$$F = \left(\frac{R'}{\Lambda}\right)^2 + \left(\frac{P_\Lambda}{R}\right)^2 \quad . \tag{6.9}$$

The Euclidean analogue of (3.7) reads then

$$\begin{aligned} P_\Lambda\delta\Lambda + P_R\delta R - P_M\delta M - P_{\mathsf{R}}\delta\mathsf{R} &= \left[R\delta R \arctan\left(\frac{\Lambda P_\Lambda}{RR'}\right)\right]' \\ &\quad + \delta\left(\Lambda P_\Lambda - RR' \arctan\left(\frac{\Lambda P_\Lambda}{RR'}\right)\right) \quad . \end{aligned} \tag{6.10}$$

There are now two ways in which one might want to proceed. On the one hand, as the Euclidean horizon is topologically just a single two-sphere, one could adopt boundary conditions that make the "spatial" slices of the Euclidean formulation end at the Euclidean horizon and fix in the variational principle the angle at the horizon, either directly or as a consequence of a horizon equation of motion. This is immediately analogous to the approach of the present paper, and the difference of the Liouville forms (6.10) can be treated as in Sec. III. The Hamiltonian reduction should therefore work in essence as in Sec. IV. On the other hand, one might want to mimic the Kruskal analysis of Kuchař and adopt boundary conditions that make one of the "spatial" slices in the Euclidean description go straight through the Euclidean horizon. In this case the identity (6.10) is more problematic, since at the horizon of the classical Euclidean solution the arctan term becomes singular in a way which prohibits one from extending the arctan to the whole Euclidean solution as a single-valued function. It is therefore not clear in what sense the Euclidean transformation from $\{\Lambda, P_\Lambda; R, P_R\}$ to $\{M, P_M; \mathsf{R}, P_{\mathsf{R}}\}$ might remain a canonical transformation if one of the spatial slices is allowed to cross the Euclidean horizon. Note that although in the Lorentzian Kruskal case of Kuchař the logarithms in (3.7) become singular at the horizons, the singularities there are integrable and do not introduce multivaluedness into the expressions.

Returning finally to our original motivations outlined in the Introduction, we have seen that although we did succeed in computing a partition function by Lorentzian Hamiltonian methods and analytic continuation, we did not recover the partition function in quite the form that was anticipated in (1.1). We did not obtain a *total* Hamiltonian that could have been multiplied by the inverse temperature and then used in (1.1). Instead, only one of the two terms in the reduced Hamiltonian can be interpreted in terms of the temperature, whereas the other term is associated with the entropy. This means that our reduced Lorentzian Hamiltonian cannot quite be identified as a quantum Hamiltonian of the kind anticipated in Refs. [16,28–31], such that the spectrum of the Hamiltonian would be given by the inverse Laplace transform of our $Z_{\rm ren}(\beta)$ [Eq. (5.11)]. In particular, the entropy of the black hole arises directly from our Hamiltonian and not from an associated density of states. One is tempted to regard this explicit appearance of the entropy in the Hamiltonian as yet another indication of the topological nature of gravitational entropy.

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APPENDIX A: TRACE REGULARIZATION

In this appendix we carry out a regularization and renormalization of the divergent trace in (5.9).[5] We work in the Hilbert space $H = L_2([0,L])$, where $L > 0$, and we denote the coordinate on $[0,L]$ by x. The L_2 inner product is denoted by $(\cdot\,,\cdot)$.

Let f be a bounded measurable function from $[0,L]$ to $\mathbb{R}$, and let $\hat{f}$ be the corresponding operator that acts on H as pointwise multiplication by f. Let $\hat{A}$ be the

[5]Using the exponential of a Laplacian as a regulator was suggested to us by Leonard Parker [62].

positive self-adjoint operator $-d^2/dx^2$ on H associated with the boundary condition that the eigenfunctions have a vanishing derivative at the boundaries $x = 0$ and $x = L$ [63]. We are interested in regularizing the divergent trace of $\hat{f}$, using the exponential of $\hat{A}$ as the regulator.

Recall first that the normalized eigenvectors ϕ_n of $\hat{A}$ are

$$\phi_0(x) = L^{-1/2},$$
$$\phi_n(x) = (2/L)^{1/2}\cos(n\pi x/L), \quad n = 1, 2, 3, \ldots, \tag{A1}$$

with the eigenvalues

$$E_n = n^2\pi^2 L^{-2} \quad , \quad n = 0, 1, 2, \ldots \ . \tag{A2}$$

Also, recall that f can be understood as a vector in H, and as such it can be expanded as

$$f = \sum_{n=0}^{\infty} f_n \phi_n \quad , \tag{A3}$$

where $f_n = (\phi_n, f)$.

Let $\alpha > 0$, and consider on H the operator

$$\hat{f}_\alpha = \exp\left(-\tfrac{1}{2}\alpha\hat{A}\right) \hat{f} \exp\left(-\tfrac{1}{2}\alpha\hat{A}\right) \quad . \tag{A4}$$

$\hat{f}_\alpha$ is bounded, and it converges to $\hat{f}$ as $\alpha \to 0$ in the strong operator topology. A straightforward computation of the trace of $\hat{f}_\alpha$ in the basis $\{\phi_n\}$ yields the finite result

$$\begin{aligned}
\mathrm{Tr}(\hat{f}_\alpha) &= \sum_{n=0}^{\infty} (\phi_n, \hat{f}_\alpha \phi_n) \\
&= \sum_{n=0}^{\infty} e^{-\alpha n^2\pi^2 L^{-2}} (\phi_n, f\phi_n) \\
&= \sum_{n=0}^{\infty} e^{-\alpha n^2\pi^2 L^{-2}} \sum_{m=0}^{\infty} f_m (\phi_n, \phi_m \phi_n) \\
&= f_0 L^{-1/2} \sum_{n=0}^{\infty} e^{-\alpha n^2\pi^2 L^{-2}} \\
&\quad + \frac{L^{-3/2}}{\sqrt{2}} \sum_{n=1}^{\infty} f_{2n} e^{-\alpha n^2\pi^2 L^{-2}} \quad .
\end{aligned} \tag{A5}$$

The term multiplying f_0 after the last equality sign in (A5) diverges at $\alpha \to 0$ as $\frac{1}{2}(L/\pi\alpha)^{1/2}$. The Riemann-Lebesgue lemma implies $\lim_{n\to\infty} f_n = 0$, and hence the second term after the last equality sign in (A5) multiplied by $\alpha^{1/2}$ goes to zero as $\alpha \to 0$. Denoting by $\mathbb{1}$ the function on $[0, L]$ which takes the constant value 1, we therefore have

$$\frac{\mathrm{Tr}(\hat{f}_\alpha)}{\mathrm{Tr}(\hat{\mathbb{1}}_\alpha)} \overset{\alpha\to 0}{\longrightarrow} L^{-1} \int_0^L dx\, f(x) \quad . \tag{A6}$$

Thus, the quantity

$$\mathrm{Tr}_{\mathrm{ren}}(\hat{f}) = L^{-1} \int_0^L dx\, f(x) \tag{A7}$$

can be understood as a renormalized trace of $\hat{f}$.

If the boundary condition for $\hat{A}$ at one end or at both ends is changed to the vanishing of the eigenfunctions, a slightly more cumbersome calculation leads to the identical result in (A6).

Note that the algebra $\mathcal{U}$ of essentially bounded measurable functions on $[0, L]$, acting on H by pointwise multiplication, is an example of an Abelian Von Neumann algebra. The renormalized trace $\mathrm{Tr}_{\mathrm{ren}}$ [Eq. (A7)] defines on $\mathcal{U}$ a faithful and finite tracial weight [64].

A similar trace renormalization has been recently employed in the context of noncommutative geometry [65,66].[6]

APPENDIX B: $\mathbb{R}P^3$ GEON: SCHWARZSCHILD HOLE WITH $\mathbb{R}P^3 \setminus \{p\}$ SPATIAL TOPOLOGY

In this appendix we describe briefly a maximal non-Kruskal extension of the exterior Schwarzschild solution known as the $\mathbb{R}P^3$ geon [37]. The geometrodynamics of the $\mathbb{R}P^3$ geon will be analyzed in Appendix C.

Recall [32,46] that the Kruskal spacetime is the pair $(\mathcal{M}, g_{ab})$, where $\mathcal{M} \simeq \mathbb{R}^2 \times S^2$ and the metric g_{ab} can be given in Kruskal coordinates as

$$ds^2 = 32M^3 R^{-1} e^{-R/2M}(-d\tilde{t}^2 + d\tilde{x}^2) + R^2 d\Omega^2 \quad , \tag{B1}$$

where $M > 0$ is the Schwarzschild mass and R is determined as a function of $\tilde{t}$ and $\tilde{x}$ from

$$-\tilde{t}^2 + \tilde{x}^2 = (R/2M - 1)e^{R/2M} \quad . \tag{B2}$$

The range of the coordinates is $\tilde{t}^2 - \tilde{x}^2 < 1$, with $\tilde{t}^2 - \tilde{x}^2 = 1$ corresponding to the past and future singularities.

Let (θ, ϕ) be the usual spherical coordinates on S^2. Consider the map $Q_0\colon (\tilde{t}, \tilde{x}, \theta, \phi) \mapsto (\tilde{t}, -\tilde{x}, \pi - \theta, \phi + \pi)$, extended by continuity to the singularities of the spherical coordinate system. Q_0 is an isometry of g_{ab}, it squares to the identity map, and its action on $\mathcal{M}$ is properly discontinuous [46]. It follows that the quotient space $\mathcal{M}' = \mathcal{M}/Q_0$ is a manifold which inherits from g_{ab} a smooth Lorentzian metric g'_{ab}. Following Ref. [37], we refer to the quotient spacetime $(\mathcal{M}', g'_{ab})$ as the $\mathbb{R}P^3$ geon.

An alternative description of the $\mathbb{R}P^3$ geon is to take the region $\tilde{x} \geq 0$ of the Kruskal spacetime and perform at the timelike boundary $\tilde{x} = 0$ the antipodal identification on S^2, $(\tilde{t}, \theta, \phi) \sim (\tilde{t}, \pi - \theta, \phi + \pi)$. One sees that $\mathcal{M}' \simeq \mathbb{R} \times (\mathbb{R}P^3 \setminus \{p\})$, and there clearly exist global 3+1 slicings of $\mathcal{M}'$ with $\mathbb{R}P^3 \setminus \{p\}$ spatial slices. The spacetime is geodesically inextendible, but it is has nevertheless only one asymptotically flat, exterior Schwarzschild region. The Penrose diagram can be found in Ref. [37]. The universal covering space is the Kruskal spacetime.

The elliptic interpretation of the Schwarzschild black hole [67], which is obtained from the Kruskal spacetime through a different quotient construction, shares with the $\mathbb{R}P^3$ geon the property that both possess only one

[6]We thank Giovanni Landi for bringing this to our attention.

exterior Schwarzschild region. However, the elliptic interpretation spacetime is space orientable but not time orientable, and the interior of the black hole is identified with the interior of the white hole. In contrast, the $\mathbb{R}P^3$ geon is both space and time orientable, and it contains separate white hole and black hole interiors behind distinct past and future horizons.

APPENDIX C: GEOMETRODYNAMICS OF THE $\mathbb{R}P^3$ GEON

The Hamiltonian analysis of spherically symmetric geometrodynamics given by Kuchař was performed under boundary conditions that in essence enforce each classical solution to be a whole Kruskal spacetime. It was found that the momentum conjugate to the Schwarzschild mass is related to the difference between what happens at the two spatial infinities. In this appendix we outline the analogous Hamiltonian analysis under boundary conditions that enforce each classical solution to be an $\mathbb{R}P^3$ geon, which has only one spatial infinity. We shall find that the Schwarzschild mass has again a canonically conjugate momentum. This momentum is now related to the difference between what happens at the single spatial infinity and at the counterpart of the Kruskal throat.

We start from the general spherically symmetric ADM metric (2.1) on $\mathbb{R}\times\mathbb{R}\times S^2$, taking now $-\infty < r < \infty$. We require N, Λ, and R to be even in r and N^r to be odd in r, and at $|r| \to \infty$ we adopt the falloff conditions of Kuchař appropriate for asymptotic flatness. The timelike three-surface $r = 0$ has then vanishing extrinsic curvature. It follows that the map Q: $(t, r, \theta, \phi) \mapsto (t, -r, \pi - \theta, \phi + \pi)$, extended by continuity to the singularities of the spherical coordinate system, is an isometry that acts properly discontinuously and squares to the identity. Taking the quotient with respect to Q yields therefore a smooth spacetime. Clearly, an alternative description of this quotient spacetime is to adopt the metric (2.1) for $0 \le r < \infty$, requiring that the even r derivatives of N^r and odd r derivatives of N, Λ, and R vanish as $r \to 0$ (possibly up to some finite order depending on the assumed degree of smoothness), and to perform at the timelike boundary $r = 0$ the identification $(t, \theta, \phi) \sim (t, \pi - \theta, \phi + \pi)$.

When the Einstein equations hold, our quotient spacetime is precisely the $\mathbb{R}P^3$ geon of Appendix B. In particular, if the Einstein equations are imposed before taking the quotient, the symmetry assumptions about $r = 0$ guarantee that $r = 0$ is a timelike surface of constant Killing time through the bifurcation two-sphere of the Kruskal spacetime. One can always choose a Kruskal coordinate system in which this timelike surface is just the surface $\tilde{x} = 0$ in the metric (B1).

Our aim is now to analyze the geometrodynamics of these quotient spacetimes. The easiest way to proceed is to follow the steps of Kuchař using the symmetry about $r = 0$ mentioned above, treating the two spatial infinities in a way which preserves the symmetry, and in the end taking the quotient. One immediately recovers the canonical geometrodynamical action in the form

$$S[\Lambda, R, P_\Lambda, P_R; N, N^r] = \int dt \int_0^\infty dr \left(P_\Lambda \dot{\Lambda} + P_R \dot{R} - NH - N^r H_r\right) - \int dt\, N_+ M_+ \quad , \tag{C1}$$

where N_+ is the asymptotic value of N at $r \to \infty$, and M_+ is determined by the asymptotic behavior of the configuration variables at $r \to \infty$ in the way explained by Kuchař. The action (C1) is appropriate for the variational principle in which $N_+(t)$ is considered fixed. It is clear how to introduce at the infinity a parameter time $\tau_+(t)$ as in Sec. III E of Kuchař, and to construct an action in which both N and τ_+ are varied freely.

The canonical transformation (3.1) with the associated redefinition of the Lagrange multipliers given by (3.3) and (3.6) yields the action

$$S[M, \mathsf{R}, P_M, P_\mathsf{R}; N^M, N^\mathsf{R}] = S_\Sigma[M, \mathsf{R}, P_M, P_\mathsf{R}; N^M, N^\mathsf{R}] \; + \; S_{\partial\Sigma}[M; N^M] \quad , \tag{C2}$$

where the surface action is given by

$$S_\Sigma[M, \mathsf{R}, P_M, P_\mathsf{R}; N^M, N^\mathsf{R}] = \int dt \int_0^\infty dr \left(P_M \dot{M} + P_\mathsf{R} \dot{\mathsf{R}} - N^M M' - N^\mathsf{R} P_\mathsf{R}\right) \quad , \tag{C3}$$

and the boundary action by

$$S_{\partial\Sigma}[M; N^M] = -\int dt\, N_+ M_+ \quad . \tag{C4}$$

In (C3), N^M is odd in r and M, R, P_M, P_R, and N^R are even in r. The falloff conditions at $r \to \infty$ are as given by Kuchař; in particular, the asymptotic values of M and N^M are, respectively, M_+ and $-N_+$. The action (C2) is appropriate for the variational principle in which $N_+(t)$ is considered fixed. Introducing at the infinity the parameter time $\tau_+(t)$, an action in which both τ_+ and N^M are varied freely is

$$S[M, \mathsf{R}, P_M, P_\mathsf{R}; N^M, N^\mathsf{R}; \tau_+] = S_\Sigma[M, \mathsf{R}, P_M, P_\mathsf{R}; N^M, N^\mathsf{R}] + S_{\partial\Sigma}[M; \tau_+] \quad , \tag{C5}$$

where

$$S_{\partial\Sigma}[M; \tau_+] = -\int dt\, M_+ \dot{\tau}_+ \quad . \tag{C6}$$

As in the paper by Kuchař, there are two ways to bring the action (C5) into Hamiltonian form. One way is to perform a standard Legendre transformation with respect to τ_+, noticing that the linearity of (C5) in $\dot{\tau}_+$ requires one to introduce a new constraint. The resulting analysis closely follows that of Kuchař, and we shall not write it out here. However, the second way of bringing

(C5) into Hamiltonian form is sufficiently different from the Kruskal case to merit a more detailed discussion.

We start from (C5). Note first that the homogeneous part of (C5) defines the one-form

$$\Theta = -M_+\delta\tau_+ + \int_0^\infty dr\, P_M(r)\delta M(r) \tag{C7}$$

on $(M(r), P_M(r); \tau_+)$. For clarity, we shall for the remainder of this appendix write explicitly out the argument of functionals of r. To cast (C7) into a Liouville form, we first split $M(r)$ into the mass at infinity m and the mass density $\Gamma(r)$, defined by

$$m = M_+ \ , \tag{C8a}$$

$$\Gamma(r) = M'(r) \ . \tag{C8b}$$

$M(r)$ is then expressed as

$$M(r) = m - \int_r^\infty dr'\, \Gamma(r') \ . \tag{C9}$$

Defining

$$p = \tau_+ + \int_0^\infty dr'\, P_M(r') \ , \tag{C10a}$$

$$P_\Gamma(r) = -\int_0^r dr'\, P_M(r') \ , \tag{C10b}$$

manipulations analogous to those of Kuchař show that Θ can be written as

$$\Theta = p\delta m + \int_0^\infty dr\, P_\Gamma(r)\delta\Gamma(r) - \delta(M_+\tau_+) \ , \tag{C11}$$

which is a Liouville form up to a total derivative. The transformation defined by (C8) and (C10) therefore brings the action (C5) to a canonical form. Finally, we perform the canonical transformation

$$T(r) = P_\Gamma(r) \ , \tag{C12a}$$

$$P_T(r) = -\Gamma(r) \ , \tag{C12b}$$

which puts Θ to the form

$$\Theta = p\delta m + \int_0^\infty dr\, P_T(r)\delta T(r) + \delta\omega \ , \tag{C13}$$

where

$$\omega = -M_+\tau_+ - \int_0^\infty dr\, M'(r) \int_0^r dr'\, P_M(r') \ . \tag{C14}$$

The action (C5) reads then

$$S_\Sigma\left[m, p; T(r), \mathsf{R}(r), P_T(r), P_{\mathsf{R}}(r); N^T(r), N^{\mathsf{R}}(r)\right]$$
$$= \int dt\, p\dot{m} + \int dt \int_0^\infty dr[P_T(r)\dot{T}(r) + P_{\mathsf{R}}(r)\dot{\mathsf{R}}(r) - N^T(r)P_T(r) - N^{\mathsf{R}}(r)P_{\mathsf{R}}(r)], \tag{C15}$$

where the multiplier $N^M(r)$ has been renamed as $-N^T(r)$, and a total derivative has been dropped. Note that $\mathsf{R}(r)$, $P_{\mathsf{R}}(r)$, and $N^{\mathsf{R}}(r)$ are even in r, whereas $T(r)$, $P_T(r)$, and $N^T(r)$ are odd in r.

The dynamical content of the actions (C5) and (C15) can now be discussed as by Kuchař. For concreteness, let us concentrate on (C15). The true dynamical degrees of freedom are the canonical pair (m, p), whereas all the other degrees of freedom are pure gauge. The true Hamiltonian vanishes, and both m and p are constants of motion. In a classical solution, m is clearly the value of the Schwarzschild mass. To understand the geometrical meaning of p, recall from Kuchař that in a classical solution the quantity $-P_M(r)$ is equal to the derivative of the Killing time with respect to r. Equations (C10b) and (C12a) then show that, in a classical solution, $T(r)$ is equal to the Killing time, with the additive constant chosen so that the Killing time vanishes on the timelike surface $\tilde{x} = 0$ in the notation of Appendix B. Now, Eq. (C10a) can be written as

$$p = \tau_+ - T(\infty) \ . \tag{C16}$$

Therefore, in a classical solution, the momentum p is the value of the parametrization time τ_+ at the asymptotic infinity on that particular spacelike surface for which the Killing time, with the zero-point chosen in the above fashion, vanishes. In the notation of Appendix B, this is the surface $\tilde{t} = 0$.

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