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Energy spectrum of a quantum black hole

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Abstract. We discuss a 'minisuperspace' path integral for the partition function of a Schwarzschild black hole in thermal equilibrium within a finite spherical box. Building on a novel classical variational principle, we define and evaluate a partition function using a non-trivial complex integration contour. The partition function solves exactly the relevant differential equation related to the Wheeler–DeWitt equation, and it has the desired semiclassical behaviour indicating in particular thermodynamical stability. For a given size of the box, the density-of-states is non-vanishing only in a finite energy interval whose upper end is twice as high as would be classically expected without negative temperatures. When negative temperatures are included, this discrepancy is resolved, and the system is then analogous to certain systems in ordinary quantum statistical mechanics which admit negative temperatures. The relation to the partition function previously obtained by Whiting and York using a Hamiltonian reduction method is discussed.

1. Introduction

It has been established for some time that the thermodynamics of asymptotically flat black hole spacetimes can be described by path integral methods [1, 2]. In recent years there has been interest in extending these path integral methods to accommodate boundary conditions that do not refer to asymptotic infinity but bring the 'boundary' to a finite distance from the hole [3–11]. The aim of this program is thus to describe a black hole in a thermal equilibrium in a finite box.

The prototype of the envisaged physical situation in Lorentzian spacetime is a radiating Schwarzschild black hole placed at the centre of a spherical box [3]. The round boundary S^2 is postulated to be mechanically rigid, yet to allow free exchange of energy between the interior and exterior of the box. The temperature measured at the boundary is postulated to be held fixed at a value which is constant all over the boundary. The parameters describing the system are thus the pair (β, A), where A is the boundary area and β is the inverse boundary temperature. These are data appropriate for the canonical thermodynamical ensemble. One would therefore expect the thermodynamics to be described by a partition function $Z(\beta, A)$. One would further expect this partition function to be obtainable from a Euclidean path

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integral, where the inverse temperature is identified as the proper circumference in the periodic Euclidean time direction. This integral would thus take the form

$$Z(\beta, A) = \int \mathcal{D}g_{\mu\nu} \exp(-I) \tag{1.1}$$

where the integration is over all metrics $g_{\mu\nu}$ within the four-dimensional 'Euclideanized' box, such that these metrics respect the fixed boundary data (β, A). The difference from the analogous path integral with boundary conditions set at the asymptotic infinity [1,2] is that the partition function (1.1) makes no reference to anything outside the finite box. In particular, β in (1.1) is the inverse temperature at the boundary, not the one measured at infinity.

A motivation for investigating the finite box partition function $Z(\beta, A)$ is that the system described by this partition function might, in contrast to a black hole in asymptotically flat space, be thermodynamically stable [3]. If the four-manifold inside the Euclideanized box is taken to be the one admitting Euclidean Schwarzschild solutions, and if β^2/A is sufficiently small, two of the saddle points of the integral (1.1) are Euclidean Schwarzschild solutions with two different values of the Schwarzschild mass†. If it is now assumed that the integral is dominated by the 'large mass' Schwarzschild saddle point, the heat capacity computed from the partition function is positive, indicating thermodynamical stability of the system. Also, the thermodynamical quantities computed from the partition function are consistent with the established asymptotically flat space results as long as the semiclassical approximation is assumed to be good; one recovers in particular the familiar Bekenstein–Hawking entropy formula [13, 14] $S \approx 4\pi M^2$.

A justification of the assumption that the path integral is dominated by the 'large mass' Schwarzschild saddle point would require a proper definition of the path integral. How to give such a definition is a notoriously open question in quantum gravity [15–18]. The issue becomes however more tractable in a simplified model where the metrics are restricted to have the symmetries of the Schwarzschild solution (spherical symmetry and staticity) throughout the interior of the box. The path integral takes then the form of that in a constrained quantum mechanical system, similar to 'minisuperspace' models familiar from quantum cosmology [19]. Although a minisuperspace ansatz like this loses most of the local degrees of freedom of the gravitational field inside the box, its invocation for the black hole partition function might be defended by the observation that it retains those global features of the geometry that are often thought of as responsible for the thermodynamical properties of black holes.

Two methods have been previously given for analysing the minisuperspace path integral for the Schwarzschild black hole partition function. The first method, by Whiting and York [5], is based on a Hamiltonian reduction of the action. This gives a manifestly convergent integral, and the resulting partition function is real-valued and has the desired semiclassical behaviour. What appears perhaps less clear is whether this partition function has all the desired properties also beyond the semiclassical regime. One issue here is that, without an unorthodox approach to the ordering question, this partition function is only an approximate solution to the differential

† Whether there exist saddle points which do not have the Schwarzschild symmetries in the interior of the box appears not known. There exists however a third saddle point with the Schwarzschild symmetries but a genuinely complex-valued metric [3, 9, 12].

equation which the path integral by construction would be expected to satisfy exactly. Another issue concerns the density-of-states computed from this partition function. This will be discussed in more detail in sections 5 and 6.

A second method for analysing this black hole minisuperspace integral, by Halliwell and Louko [12], was based on Hartle's suggestion [20] of using steepest-descent contours for finding and enumerating general complex contours of integration [21–27]. This method amounted in essence to assuming that the only non-trivial contour structure lies in the Lagrange multiplier associated with the radial constraint in the minisuperspace action, and the convergent contours in this Lagrange multiplier were then analysed in some detail. It was however found difficult to recover with this method a partition function which would be real-valued and get its dominant contribution from the thermodynamically desirable 'large mass' Schwarzschild saddle point.

The purpose of the present paper is to give a new method for defining and evaluating the minisuperspace path integral for the Schwarzschild black hole partition function. Our method combines elements from both of the previous analyses, but it uses as its starting point a novel way of looking at the classical variational principle whose boundary data are those of the path integral. We shall recover a partition function which is an exact solution to the expected differential equation, and this partition function will share the desirable thermodynamical properties of the amplitude obtained by Whiting and York. The density-of-states computed from the partition function turns out to be non-vanishing in an energy range which, for fixed size of the box, is bounded both from above and below. The lower bound on the energy is at zero, as expected by the classical positive energy theorems, but the upper bound is twice as high as would have been expected by purely classical considerations for positive temperatures. This indicates a close analogy between the black hole energy spectrum and that occurring in certain spin systems familiar from ordinary statistical mechanics. These results are in agreement with but go further than the semiclassical analysis of the density-of-states given in [4].

We begin in section 2, after introducing the model and establishing the notation, by presenting a new classical variational principle consistent both with the minisuperspace dynamics and with the boundary data of the anticipated path integral. In section 3 we build a path integral on this variational principle, relying in part on previous work on the integration contours [12]. The density-of-states is evaluated in section 4. Section 5 contains a discussion of the thermodynamical properties of the partition function and the density-of-states, and a comparison with the earlier work. The results are summarized and discussed in section 6.

2. *The classical variational principle*

We consider metrics of the form

$$\mathrm{d}s^2 = N^2(y)\mathrm{d}y^2 + a^2(y)\mathrm{d}\chi^2 + b^2(y)\mathrm{d}\Omega^2 \tag{2.1}$$

where $\mathrm{d}\Omega^2$ is the metric of the unit two-sphere and the coordinate χ is periodic with period 2π. We take these metrics to be defined on the manifold $\mathcal{M} = \bar{D} \times S^2$, where $\bar{D}$ is the closed two-dimensional disc. This is achieved by letting the range of the coordinate y to be (without loss of generality) $0 < y \leqslant 1$, and interpreting (y, χ) as a polar coordinate system on the disc with $y = 0$ being the coordinate singularity at the centre. The coordinates in the ansatz thus cover all of $\mathcal{M}$ except the centre S^2 at $y = 0$. Note that for the Euclidean Schwarzschild solution, which is contained among our metrics as a special case, the coordinate χ is proportional to the periodically identified Euclidean time [1].

Our manifold $\mathcal{M}$ is compact with a boundary $\partial\mathcal{M} = S^1 \times S^2$, located at $y = 1$. We are interested in the classical boundary value problem where the boundary data consists of the intrinsic metric on $\partial\mathcal{M}$. With our ansatz these data amount to giving the boundary values of the two 'scale factors' $a(1)$ and $b(1)$. In the thermodynamical interpretation in terms of the boundary data in the partition function (1.1), this means fixing the boundary area to $4\pi b^2(1)$ and the boundary inverse temperature to $2\pi a(1)$. The solutions to this boundary value problem are sections of the Schwarzschild solution, with the Schwarzschild mass given as a triple-valued function of the boundary data. Two of the solutions may be either real Euclidean or a complex conjugate pair, depending on whether $[a(1)/b(1)]^2$ is smaller or larger than $\frac{16}{27}$. The third solution is always genuinely complex [3, 9, 12].

A variational formulation of this boundary value problem is well known. In general, the action appropriate for fixing the intrinsic metric on $\partial\mathcal{M}$ is the modified Einstein–Hilbert action [1, 28], given in Planck units by

$$I = -\frac{1}{16\pi}\int_{\mathcal{M}} R - \frac{1}{8\pi}\int_{\partial\mathcal{M}} (K - K_0) \tag{2.2}$$

where K is the trace of the extrinsic curvature tensor on $\partial\mathcal{M}$ and K_0 is the trace of the extrinsic curvature tensor that $\partial\mathcal{M}$ would have were it embedded in flat Euclidean space. Although K_0 does not exist for arbitrary three-metrics on $\partial\mathcal{M}$, it is well defined for metrics within our class. Inserting the ansatz (2.1) into the action gives a 'minisuperspace' action of the form

$$I = \int_0^1 L\,\mathrm{d}y + (\text{boundary terms}) \tag{2.3}$$

where the Lagrangian is given by

$$L = \pi N\left(-\frac{ab'^2 + 2ba'b'}{N^2} - a\right). \tag{2.4}$$

Here the prime stands for derivative with respect to y. When the coordinate singularity at $y = 0$ and the boundary terms in (2.3) are carefully treated, the variation of the action is well known to lead to the full Einstein equations for our ansatz, and the stationary configurations are the solutions to our boundary value problem on $\mathcal{M}$ [5, 12, 29, 30].

The delicate issue in this variational principle is the coordinate singularity at $y = 0$. At the purely classical level such coordinate singularities are not especially problematic, since one would usually define the class of metrics in which the action is to be varied in a coordinate-invariant way. In particular, one would usually take the metrics to belong to some appropriate differentiability class on $\mathcal{M}$, such as C^2 or C^∞; what this in practice implies for the metrics within our ansatz has been discussed in some detail in [12, 30]. If however one wishes to pass from the classical level to the quantum level and use the variational principle for constructing a path integral, the coordinate singularity calls for more attention.

The heart of the problem is that the minisuperspace action (2.3) has the appearance of an action in a quantum mechanical system with y playing the role of 'time.' When building a path integral on such an action, one is compelled to discuss whether some kind of boundary data should be given in the integral not only at the actual boundary of the manifold at $y = 1$, but also at the 'centre' of the manifold at $y = 0$. A number of different sets of boundary conditions for this situation have been introduced, all of them presenting data which maintain consistency at the level of the variational principle but which would also be expected to admit a consistent implementation in the path integral [5, 12, 29, 30].

We shall now introduce a new set of boundary conditions of this kind, and we demonstrate its consistency at the level of the variational principle. We are not aware of arguments which would prefer this set of conditions over those given in the previous literature purely at the level of the variational principle. Our motivation is that this data set will allow us to construct in section 3 a path integral with properties expected of a black hole partition function. The relation to path integrals constructed from other classically equivalent data sets will be discussed in section 6.

Begin by considering the action

$$I = \int_0^1 L\,\mathrm{d}y + 2\pi a(1)b(1) - \pi b^2(0) \tag{2.5}$$

where L is given by (2.4). For metrics that are C^2 on $\mathcal{M}$, it is easily shown that this action is equal to the 'full' action (2.2). However, we are striving for a variational principle which would *not* refer to statements about the four-dimensional differentiability on $\mathcal{M}$, but rather to some appropriate 'initial' conditions at $y = 0$. We shall therefore, for the moment, take (2.5) as a definition. The relation to the full action (2.2) will be discussed at the end of this section.

We take the action (2.5) to be defined on sufficiently smooth (say C^2) functions $a(y)$, $b(y)$ and $N(y)$ for $0 \leqslant y \leqslant 1$. (Note that we thus do not at this stage require smoothness of the metrics at the coordinate singularity at $y = 0$ on $\mathcal{M}$.) The boundary conditions imposed at $y = 0$ and $y = 1$ are taken to be the following:

$$a(1), b(1) \qquad \text{fixed} \tag{2.6a}$$

$$a(0) = 0\,. \tag{2.6b}$$

The conditions at $y = 1$ are as expected. It is in the condition at $y = 0$ that we differ from previous work. A closely related set of conditions has been discussed in [30].

We can now investigate the action (2.5) by varying it under the conditions (2.6). After integrations by parts, with careful attention to the boundary terms, we obtain

$$\delta I = \int_0^1 \left[\left(\frac{\delta L}{\delta a}\right)\delta a + \left(\frac{\delta L}{\delta b}\right)\delta b + \left(\frac{\partial L}{\partial N}\right)\delta N \right] \mathrm{d}y + \pi \left[\left(\frac{a'}{N} - 1\right)\delta(b^2) \right]_{y=0} \tag{2.7}$$

where $\delta L/\delta a$ is the usual Euler–Lagrange variational derivative,

$$\frac{\delta L}{\delta a} \equiv \frac{\partial L}{\partial a} - \frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{\partial L}{\partial a'}\right) \tag{2.8}$$

and similarly for $\delta L/\delta b$. As the two terms in δI are independent and the value of $b(0)$ is not fixed in the variation, the equations that follow from setting δI to zero are the usual Euler–Lagrange equations

$$\frac{\delta L}{\delta a} = \frac{\delta L}{\delta b} = \frac{\partial L}{\partial N} = 0 \tag{2.9}$$

and the equation

$$\frac{a'}{N} = 1 \qquad \text{at } y = 0\,. \tag{2.10}$$

The Euler–Lagrange equations (2.9) are well known to be equivalent to the Einstein equations for our metric ansatz where the coordinate system used in the ansatz is non-singular [31]. It can now be verified [12, 30] that the conditions (2.6*b*) and (2.10) enforce the solutions to the Euler–Lagrange equations (2.9) to behave near $y = 0$ so that these metrics are in fact solutions to the Einstein equations on our full manifold $\mathcal{M} = \bar{D} \times S^2$, with $y = 0$ just a coordinate singularity at the centre of the disc. In other words, our variational principle leads to the solutions of the boundary value problem on $\mathcal{M}$ that we are interested in. This variational principle could thus be expected to give a viable starting point for a path integral construction.

The subtlety that remains is the relation between the minisuperspace action (2.5), which we have taken here as a definition, and the full action (2.2). As mentioned above, these actions are equal for metrics that are C^2 on $\mathcal{M}$. In particular, they are equal for the classical solutions recovered from the variational principle, since these solutions are regular sections of the Schwarzschild solution and thus in fact analytic. It can also be shown that the two actions agree for metrics that satisfy (2.6*b*) while having no worse than conical singularities at $y = 0$ [30]. For generic metrics within our ansatz that are assumed to satisfy just (2.6*b*), however, it is difficult to ascertain what the relation between the two actions is, or even whether the full action (2.2) can be meaningfully defined [32].

Thus, although our minisuperspace variational principle is a consistent one for recovering the classical solutions, it remains at present open what its relation to the full action (2.2) is for all the non-extremal metrics that are included in the variations. This issue appears to arise in different guises in all the previous variational principles that avoid referring to the differentiability of the four-dimensional metrics at the coordinate singularity [5, 12, 29, 30].

3. Path integral for the partition function

A path integral based on the variational principle presented in the previous section takes the form

$$Z(\beta, r_0) = \int_{a(0)=0}^{\substack{2\pi a(1)=\beta \\ b(1)=r_0}} \mathcal{D}N\mathcal{D}a\mathcal{D}b \exp(-I)\,. \tag{3.1}$$

The boundary data (2.6*a*) have been written in terms of the thermodynamical interpretation of Z as a black hole partition function. The area of the boundary two-sphere is $4\pi r_0^2$, and β is the inverse temperature at the boundary.

We shall now describe our choice for the path measure in (3.1) and evaluate the resulting partition function. Some ingredients in our choice are dictated by internal consistency, but the ulterior guiding principle is in the properties of the amplitude obtained. This logic is similar to using the predictions for Lorentzian spacetimes as a guiding principle for choosing the contour in quantum cosmological path integrals [12, 20–27].

A first question is how to treat the unconventional initial data at $y = 0$. If we envisage the integral to be defined as a limit of discretizations in y, the condition (2.6b) in the discretized integrals would formally amount to fixing $a(0)$ to zero but integrating over $b(0)$. After passing to the limit, one might expect to obtain

$$Z(\beta, r_0) = \int \mu(r_+)\, \mathrm{d}r_+\, G(\beta/2\pi, r_0; 0, r_+) \tag{3.2}$$

where the amplitude G is defined as

$$G(a'', b''; a', b') = \int_{\substack{a(0)=a' \\ b(0)=b'}}^{\substack{a(1)=a'' \\ b(1)=b''}} \mathcal{D}N \mathcal{D}a \mathcal{D}b \exp(-I)\,. \tag{3.3}$$

In (3.2) we have chosen the factor $\mu(r_+)$ to be a function of only r_+, but in principle it is a measure which could depend on the details of the discretization. This approach is admittedly hazardous, and there might even exist path measures for which the passage from (3.1) to (3.2) cannot be justified. For example, one might be using a path measure for which a and b can no longer be considered independent good coordinates at the limit $a \to 0$. We nevertheless now adopt (3.2) as the definition of (3.1), and proceed to fix the further elements that need to be specified in (3.2).

We focus next on the amplitude $G(a'', b''; a', b')$. As the boundary terms in the action (2.5) are functions of the values of a and b at $y = 0$ and $y = 1$ only, these terms factorize out of G, and what remains is just a standard propagation amplitude between two three-surfaces with fixed intrinsic three-metrics. Such amplitudes have been extensively studied in quantum cosmology [12, 21–25, 33–39].

With our action, one class of conceivable definitions of G was discussed in [12]. In the method used therein, the (radial) lapse-function $N(y)$ was first rescaled by a factor of $1/a$, and the gauge freedom was eliminated by going to the 'proper-time' gauge with respect to the new rescaled lapse. The $\mathcal{D}a\mathcal{D}b$ integrals reduced to pure Gaussians, for which convergent contours could be found and which could then be evaluated. The measure in the $\mathcal{D}a\mathcal{D}b$ integration was chosen to be compatible with the Laplacian ordering in the Dirac quantized theory [37, 40, 41]. The remaining integral over the gauge-fixed rescaled N was then analysed by the method of steepest descents, and the amplitudes obtained by different integration contours were evaluated. For the details, and for discussion of the possible caveats in this method, see [12].

In this paper, we also choose our G to be defined using the method of [12], with the contour for the rescaled N being a closed loop around $N = 0$. Up to numerical factors which can be absorbed into the measure, this gives

$$G(a'', b''; a', b') = \exp(-2\pi a'' b'' + \pi b'^2)\, I_0\left[2\pi\sqrt{\left(b'' a''^2 - b' a'^2\right)(b'' - b')}\right] \tag{3.4}$$

where I_0 is a modified Bessel function [42]. (Note that our a and b differ from those in [12] by a factor of $\sqrt{2\pi}$.) In spite of the square root in (3.4), G is an analytic function of its arguments everywhere in the finite complex domain, since I_0 is an even analytic function in the finite complex plane. The partition function can thus be written as

$$Z(\beta, r_0) = \exp(-\beta r_0) \int \mu(r_+)\,\mathrm{d}r_+\, I_0\left[\beta r_0 \sqrt{1-(r_+/r_0)}\right] \exp\left(\pi r_+^2\right) . \tag{3.5}$$

What remains is the $\mathrm{d}r_+$ integral in (3.5). In the spirit of general complex contours, and considering that the $\mathcal{D}a\mathcal{D}b$ contours and the $\mathcal{D}N$ contour were already complex, it might seem appealing to look for complex contours also for r_+. If the measure $\mu(r_+)$ is assumed to be slowly varying, the dominating term in the integrand in (3.5) at large $|r_+|$ is the exponential, and non-trivial infinite convergent contours for r_+ do exist. If $\mu(r_+)$ in particular incorporates no non-trivial complex structure, such as poles or branch cuts, all these infinite convergent contours are equivalent to integrating r_+ along the imaginary axis from $-\mathrm{i}\infty$ to $+\mathrm{i}\infty$. However, the partition function obtained from this contour is dominated by the thermodynamically unstable 'low mass' saddle point [3]. As it would appear that semi-infinite contours lead to complex-valued partition functions, we are therefore enforced to look for alternative, finite contours.

Let us choose to integrate r_+ along the real axis between some lower and upper limits f_1 and f_2, which we allow to depend on r_0. For convergence, both f_1 and f_2 must be finite. We seek to determine whether acceptable values of f_1 and f_2 exist. We shall throughout assume $\mu(r_+)$ to be so smooth and slowly varying that it will not play an essential role in the analysis.

A first constraint is that we wish the partition function, at least for some values of the boundary data, to be dominated by the 'large mass' saddle point, which resides in the interval $\frac{2}{3}r_0 \leqslant r_+ < r_0$ when it exists. We therefore need $f_1 \leqslant \frac{2}{3}r_0$ and $f_2 \geqslant r_0$. On the other hand, the f must not be so far out that the exponential term in the integrand would cause the dominating contribution to be that picked from near $r_+ \approx f_1$ or $r_+ \approx f_2$.

A second constraint arises from demanding that the partition function satisfy the differential equation which, by construction, it should satisfy [33–35, 39]. Defining

$$Z(\beta, r_0) = \exp(-\beta r_0)\, \Psi(\beta, r_0) \tag{3.6}$$

and transforming from the 'coordinates' (β, r_0) to a new pair (s_0, r_0) where $s_0 = \beta^2 r_0$, this differential equation is [12]

$$\left(4\frac{\partial^2}{\partial s_0\, \partial r_0} - 1\right) \Psi = 0 . \tag{3.7}$$

The exponential factor between Z and Ψ comes just from the K_0 term in the action (2.2), and in the cosmological context (3.7) would be understood as the Wheeler–DeWitt equation and Ψ as the wavefunction of the Universe. The covariant Laplacian ordering has been chosen. (Note that in our case of two degrees of freedom this ordering is invariant under lapse rescalings [37, 41].) Inserting (3.5) into (3.7), we find

$$f_2 = r_0 \qquad \text{or} \qquad \frac{\mathrm{d}f_2}{\mathrm{d}r_0} = 0 \tag{3.8}$$

and a similar set of conditions for f_1. To satisfy this and still guarantee that the 'large mass' saddle point dominates, we must take $f_2 = r_0$ and make f_1 independent of r_0, and further make $|f_1|$ at most of the order of unity. (Note that Planck length equals 1 in our units.) Here we shall take $f_1 = 0$ and postpone the discussion of non-zero values of f_1 until the next section. The final expression for our partition function becomes then

$$Z(\beta, r_0) = \exp(-\beta r_0) \int_0^{r_0} \mu(r_+)\, \mathrm{d}r_+\, I_0 \left[\beta r_0 \sqrt{1-(r_+/r_0)}\right] \exp\left(\pi r_+^2\right) . \qquad (3.9)$$

As will be discussed in more detail in section 5, the leading semiclassical behaviour of (3.9) is closely similar to that of the partition function obtained by Whiting and York. The differences are more significant for the density-of-states, which will be computed in the next section.

A way to characterize our partition function (3.9) is to notice that the Wheeler–DeWitt equation (3.7) is a hyperbolic differential equation, with (s_0, r_0) a pair of null coordinates. The future light cone of the origin is a characteristic surface, and any solution inside the future light cone whose limiting values on the light cone are sufficiently regular can be uniquely recovered from these limiting values. For the Ψ that corresponds to our partition function (3.9), the limiting values on the r_0 axis are determined by the measure $\mu(r_+)$, and the limiting values on the s_0 axis are vanishing. This means that our expression (3.9), independently of our having arrived at it from a path integral, contains with some $\mu(r_+)$ every partition function which is consistent with the Wheeler–DeWitt equation, has a sufficiently regular limit on the light cone, and vanishes on the s_0 axis. The path integral origins of (3.9) are nevertheless required in order to suppose something about the properties of $\mu(r_+)$, such as that it should be a slowly varying function.

With our smoothness assumptions, this characterization in terms of characteristic boundary data means that our $Z(\beta, r_0)$ can be uniquely recovered from its high-temperature limit $\beta \to 0$ using the Wheeler–DeWitt equation, provided we know also that $Z(\beta, r_0)$ vanishes at the double limit of $r_0 \to 0$ and $\beta \to \infty$ such that $\beta^2 r_0$ remains finite. Notice that the double limit condition would need to be modified if f_1 had been chosen to be non-zero.

4. Density of states

In ordinary quantum statistical mechanics, the partition function of a canonical ensemble would emerge from the Hamiltonian formalism as

$$Z(\beta) = \mathrm{Tr}\left(\exp(-\beta \hat{H})\right) \qquad (4.1)$$

where $\hat{H}$ is the Hamiltonian operator and the trace is taken in the appropriate Hilbert space. Taking the trace in a basis of energy eigenstates one obtains

$$\begin{aligned} Z(\beta) &= \sum_{\text{states}} \mathrm{e}^{-\beta E} \\ &= \int \mathrm{d}E\, \nu(E)\, \mathrm{e}^{-\beta E} \end{aligned} \qquad (4.2)$$

where the density-of-states $\nu(E)$ contains the information about the distribution of the energy eigenstates as a function of the energy E. Note that this encompasses both continuous and discrete spectra; in the latter case $\nu(E)$ would consist of delta-function peaks at the eigenenergies.

In the black hole case, a Hamiltonian expression analogous to (4.1) for the partition function is not known. Nevertheless, having at hand a partition function obtained directly from a path integral, we invert the above reasoning and, following [3–5], seek for a density-of-states $\nu(E, r_0)$ which satisfies

$$Z(\beta, r_0) = \int \mathrm{d}E\, \nu(E, r_0)\, \mathrm{e}^{-\beta E}\,. \tag{4.3}$$

Such a density-of-states could be interpreted as containing the information about the distribution of the the quantum energy eigenvalues of the black hole system.

The integral in (4.3) has the form of a Fourier–Laplace transform in E. If $\nu(E, r_0)$ satisfying this equation exists, it can be recovered from $Z(\beta, r_0)$ as the Bromwich integral

$$\nu(E, r_0) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma} \mathrm{d}\beta\, \mathrm{e}^{\beta E}\, Z(\beta, r_0) \tag{4.4}$$

where, since $Z(\beta, r_0)$ has no singularities in the finite complex β plane, the contour Γ can be chosen to be the imaginary β axis. Inserting (3.9) into (4.4), interchanging the order of the integrations and performing the dβ integral [42], we obtain

$$\nu(E, r_0) = \begin{cases} 0 & \text{for } E \leqslant 0 \\ (1/\pi) \displaystyle\int_0^{2E-(E^2/r_0)} \mu(r_+)\, \mathrm{d}r_+ \frac{\exp\left(\pi r_+^2\right)}{\sqrt{r_0(r_0 - r_+) - (E - r_0)^2}} & \text{for } 0 \leqslant E \leqslant 2r_0 \\ 0 & \text{for } E \geqslant 2r_0\,. \end{cases} \tag{4.5}$$

This expression for $\nu(E, r_0)$ satisfies (4.3), and it therefore does give the density-of-states sought for. This can be directly verified by substituting (4.5) into (4.3), interchanging the order of the integrations and performing the dE integral [42].

It is useful to rewrite $\nu(E, r_0)$ as

$$\nu(E, r_0) = \begin{cases} \dfrac{1}{\pi} \sqrt{\dfrac{2M}{r_0}} \displaystyle\int_0^1 \frac{\mu(2Mx)\, \mathrm{d}x}{\sqrt{1-x}} \exp\left(4\pi M^2 x^2\right) & \text{for } M > 0 \\ 0 & \text{for } M \leqslant 0 \end{cases} \tag{4.6}$$

where $M(E, r_0)$ is the mass of a classical Schwarzschild black hole in terms of the energy and size of the system [3,4],

$$M(E, r_0) = E - \frac{E^2}{2r_0}\,. \tag{4.7}$$

It is interesting that although our expression (4.6) arose from a path integral, the assumptions that the partition function be a Laplace transform by (4.3) and that it be related to a solution to the Wheeler–DeWitt equation (3.7) by (3.6) can be shown to imply, quite independently of any path integral considerations, that $\nu(E, r_0)$ must be of the form $r_0^{-1/2} F(M(E, r_0))$ for some function F. Further properties of our density-of-states will be considered in section 5.

If the quantity f_1 introduced in section 3 had been taken to be non-zero but at most of order unity, the density-of-states would still be qualitatively similar to (4.5). The lower limit of the r_+ integral would just be replaced by f_1, and this would shift the upper and lower limits of the energy range where the density-of-states is non-vanishing slightly away from $E = 0$ and $E = 2r_0$, that is, from $M = 0$.

5. Thermodynamical properties and comparison to the reduction method

We shall now investigate closer the thermodynamical properties of our partition function and density-of-states. We assume throughout the measure $\mu(r_+)$ to be so smooth and slowly varying that its precise properties will not be essential for the semiclassical behaviour. We assume in particular $\mu > 0$ for $r_+ > 0$.

When $r_0 \gg 1$ and $\beta \gg 1$, which is the domain relevant for physics far below the Planck regime, the integral (3.9) gets its dominant contribution from values of r_+ at which the argument of I_0 is large and positive. Replacing I_0 by the first term in its asymptotic expansion at large positive argument [42] one recovers

$$Z(\beta, r_0) \approx \frac{\exp(-\beta r_0)}{\sqrt{2\pi\beta r_0}} \int_0^{r_0} \frac{\mu(r_+)\,\mathrm{d}r_+}{[1-(r_+/r_0)]^{1/4}} \exp\left(\beta r_0 \sqrt{1-(r_+/r_0)} + \pi r_+^2\right). \tag{5.1}$$

This can be compared to the partition function

$$Z_{\mathrm{WY}}(\beta, r_0) = \exp(-\beta r_0) \int_0^{r_0} \tilde{\mu}(r_+)\,\mathrm{d}r_+ \exp\left(\beta r_0 \sqrt{1-(r_+/r_0)} + \pi r_+^2\right) \tag{5.2}$$

which was obtained by Whiting and York by the method of Hamiltonian reduction [5]. Here $\tilde{\mu}(r_+)$ is a pre-exponential measure. The semiclassical techniques used for analysing $Z_{\mathrm{WY}}(\beta, r_0)$ in [5,7] are readily applicable to (5.1), the only differences resulting from the specific choice $\tilde{\mu}(r_+) = r_+$ made in [5,7] and from the prefactor $\beta^{-1/2}$ in (5.1). Recalling that the energy expectation value $\langle E \rangle$ and the heat capacity C_{r_0} are defined by

$$\langle E \rangle = -\frac{\partial}{\partial\beta} \ln Z \tag{5.3}$$

$$C_{r_0} = \beta^2 \frac{\partial^2}{\partial\beta^2} \ln Z \tag{5.4}$$

one sees that the prefactor $\beta^{-1/2}$ in (5.1) has no effect on C_{r_0}, and its only effect in $\langle E \rangle$ is a shift of order unity which becomes irrelevant in the semiclassical analysis. One thus recovers essentially the same results about the behaviour of $\langle E \rangle$ and the positivity of the heat capacity C_{r_0} as in [5,7]. For $\beta/r_0 < \frac{32}{27}\pi$, $Z(\beta, r_0)$ is dominated by the 'large mass' Euclidean Schwarzschild solution. For $\beta/r_0 > \frac{32}{27}\pi$, on the other hand, $Z(\beta, r_0)$ is not dominated by any saddle point but by contributions from $r_+ \approx 0$.

From the exact expressions (3.9) and (5.3), it is seen using known properties of the Bessel functions [42] that the energy expectation value satisfies

$$0 < \langle E \rangle < r_0 \tag{5.5}$$

for all $r_0 > 0$ and $0 < \beta < \infty$, including the Planck regime. The limiting values 0 and r_0 in (5.5) are approached asymptotically at $\beta \to \infty$ and $\beta \to 0$, respectively. Also, as the density-of-states is always positive by our assumptions, it follows from the expression of the partition function as a Laplace transform that C_{r_0} remains positive for all $r_0 > 0$ and $0 < \beta < \infty$, including the Planck regime.

Let us now turn to the density-of-states $\nu(E, r_0)$ (4.5). When viewed as a function of E at fixed r_0, our $\nu(E, r_0)$ shows that the energy spectrum is bounded from below by $E = 0$ and from above by $E = 2r_0$. In terms of the classical configurations of the system these bounds can be understood as follows. When the classical boundary value problem for positive β and r_0 has a solution which is a positive definite metric, the corresponding E satisfies $0 < E < r_0$, and M given by (4.7) is just the mass of the classical Schwarzschild black hole. However, in accord with the partition function and density-of-states which we have constructed, there is no loss of compatibility in formally extending the classical boundary value problem with given β and r_0 and the classical relation between E and β to negative values of β. As β appears in the metric only through its square, the classical solutions will be the same metrics for positive and negative β, but for negative β it turns out that E for positive definite metrics satisfies $r_0 < E < 2r_0$ and M given by (4.7) still obeys $0 < M < r_0/2$ and has the same meaning as above. In fact, behaviour of the kind which this entails is familiar from certain spin systems in ordinary quantum statistical mechanics [43], where the high energy part of the spectrum, which is cut off from above, is formally associated with negative temperatures. That a similar interpretation in the black hole situation might be possible, is supported by the observation that $Z(\beta, r_0)$ as given by (3.9) is also finite for all negative values of β. The energy expectation values have the symmetry $\langle E \rangle \to 2r_0 - \langle E \rangle$ as $\beta \to -\beta$, so the expectation values in the range $r_0 < \langle E \rangle < 2r_0$ are formally recovered if one allows negative temperatures. It is however not clear whether it would be physically feasible to prepare a black hole system in such a negative temperature state.

We see from (4.6) that for all situations in which M is large ($M \gg$Planck mass), we have

$$\nu(E, r_0) \sim \exp(4\pi M^2) \tag{5.6}$$

where the pre-exponential factor depends on the details of the measure $\mu(r_+)$ near $r_+ \approx 2M$. In (5.6), the exponent is the expected Bekenstein–Hawking entropy of the black hole. At the limits $E \to 0$ and $E \to 2r_0$, where $M \to 0$, the behaviour of $\nu(E, r_0)$ is dictated by the details of the measure $\mu(r_+)$ near $r_+ = 0$. If for example $\mu(r_+) \xrightarrow{r_+ \to 0} r_+^p$, $p > -1$, we have

$$\nu(E, r_0) \approx \frac{(2M)^{p+1/2}}{\sqrt{\pi r_0}} \frac{\Gamma(p+1)}{\Gamma(p+(3/2))}. \tag{5.7}$$

We saw above that the semiclassical behaviour of $Z_{\mathrm{WY}}(\beta, r_0)$ and our partition function are closely similar. The differences however become more marked when comparing the energy spectra. The density-of-states corresponding to $Z_{\mathrm{WY}}(\beta, r_0)$ is [5]

$$\nu_{\mathrm{WY}}(E, r_0) = \begin{cases} 0 & \text{for } E < 0 \\ 2\tilde{\mu}(2M)\left(1 - \dfrac{E}{r_0}\right)\exp\left(4\pi M^2\right) & \text{for } 0 \leqslant E \leqslant r_0 \\ 0 & \text{for } E \geqslant r_0 \end{cases} \tag{5.8}$$

In the domain $0 < E < r_0$, where solutions to the classical boundary value problem exist for $\beta > 0$, $\nu_{\mathrm{WY}}(E, r_0)$ and our $\nu(E, r_0)$ qualitatively agree except very close to $E = r_0$, where ν_{WY} falls rapidly to zero. However, in the domain $r_0 < E < 2r_0$, where our density-of-states indicated the existence of negative temperature states, ν_{WY} is identically vanishing.

A way of modifying $Z_{\mathrm{WY}}(\beta, r_0)$ to give a non-vanishing density-of-states for $E > r_0$ would be to add to (5.2) a similar contribution in which the sign of the square root in the exponent is the opposite. In the domain relevant for physics much below Planck scale the added piece would be exponentially suppressed, and the thermodynamical expectation values computed from the partition function would thus remain essentially unchanged. The resulting density-of-states would coincide with (5.8) for $E \leqslant r_0$ and $E \geqslant 2r_0$, but for $r_0 \leqslant E < 2r_0$ it would be given by

$$2\tilde{\mu}(2M)\left(\frac{E}{r_0} - 1\right)\exp\left(4\pi M^2\right) . \tag{5.9}$$

This would give qualitative agreement with our $\nu(E, r_0)$ (4.5) everywhere except very close to $E = r_0$.

It is however not clear how a modification of this kind could be justified purely within the Hamiltonian reduction method. In particular, this modification cannot be reproduced by making the r_+ integral in (5.2) into a complex contour integral from $r_+ = 0$ around $r_+ = r_0$ and back to $r_+ = 0$, such that the square root would have a negative sign on the way back. The reason is that this contour integral would give the two contributions with opposite signs, and (5.9) would therefore get replaced by its negative.

6. Conclusions and discussion

In this paper we have discussed a path integral description of a Schwarzschild black hole in thermal equilibrium within a finite spherical box. We considered a 'minisuperspace' type model in which the metrics are restricted to be spherically symmetric and static throughout the interior of the box. Following earlier work on the boundary value problem which corresponds to fixing the 'size' of the box and the temperature measured at the boundary of the box, we formulated first a new kind of a classical variational principle, and we then elevated this variational principle into a path integral giving a partition function for the system. With a suitably chosen measure, we recovered a partition function which is an exact solution to the expected differential equation and whose thermodynamical properties far below Planck scale are closely similar to those of the partition function previously obtained for this problem by Whiting and York, using a method of Hamiltonian reduction in the path integral. The density-of-states was found to behave asymptotically as the exponential of the Bekenstein–Hawking entropy, and for a given size of the box the density-of-states was found to be non-vanishing only in a finite energy interval. The lower end of this interval was at zero, as anticipated by the positive energy theorems of the classical theory, but the upper end was twice as high as what would have been expected by purely classical considerations, without the inclusion of negative temperatures. This demonstrates a close analogy between the black hole density-of-states and that of certain spin systems in ordinary quantum statistical mechanics. In particular, the high energy end of the spectrum corresponds to thermal states which are formally associated only with negative temperatures.

The boundary data in the classical variational principle adopted in section 2 may at first sight seem surprising. If our minisuperspace model is viewed as a Lagrangian system with the radial coordinate y playing the role of time, one might have expected to fix in the variational principle two pieces of initial data and two pieces of final data. The subtleties arose from the fact that this Lagrangian system was to describe metrics on a manifold on which the initial value of y is geometrically not a boundary, but a singularity of the $(3+1)$ slicing at the 'centre' of the manifold. We found a self-consistent variational principle which superficially fixes only one piece of initial data at the initial value of y. We were however not able rigorously to demonstrate what the relation is between the minisuperspace action used in this variational principle and the corresponding full action of general relativity, the reason being that our variational principle includes some rather singular (non-extremal) metrics for which the definition of the full action of general relativity becomes a very delicate question. Similar observations concerning the coordinate singularity at the initial value of y have been made also with the variational principles previously considered for this problem [5, 12, 29, 30].

When building in section 3 a path integral on the classical variational principle, we chose to implement the unconventional initial data by integrating over the scale factor b whose initial value was not fixed in the variational principle. Formally, one might expect this to be equivalent to fixing something related to the conjugate momentum of b. Indeed, if one chooses the new coordinates $A = b^2$ and $B = ab$, one finds that the conjugate momenta are $P_A = -\pi a'/N$ and $P_B = -2\pi b'/N$ [12, 29]. Therefore our initial data could be understood as setting $B = 0$ and integrating over A, which by the term $-\pi A(0)$ in the action (2.5) could be expected to be equivalent to setting $P_A = -\pi$, or $a'/N = 1$. These were the data adopted in [12]. However, the method used in defining the integral in [12] led to a partition function differing from that of ours. This underscores explicitly that although amplitudes with different classically equivalent initial data sets might naively seem equivalent by a Fourier–Laplace type transformation, an actual demonstration of such an equivalence would require a careful definition of the respective path integrals in a way compatible with the Fourier–Laplace transforms. One would in particular need to specify the contours of the path integrals in a way compatible with the contours of the transforms.

When defining the path integral in section 3, one guideline for choosing the details of the path measure and the contours of integration was in the semiclassical properties we anticipated the result to have. This is very similar to using predictions for Lorentzian spacetimes as a guiding principle for choosing the measure and the contour in quantum cosmological path integrals [12, 20–27]. Our second guideline was that the partition function should satisfy a differential equation which, up to the K_0 normalization term in the action, is the familiar Wheeler–DeWitt equation. This deserves a comment.

Ideally, one would like to start by defining the path measure in full detail, including the ranges of all the integration variables and the contours of integration, and only after that to derive a differential equation which the propagation amplitude or wave-function or partition function satisfies. This is the approach taken in the derivations of the Wheeler–DeWitt equation under the conditions adopted in [33–35,37,39]. It is widely believed that a path integral for our geometrical situation should, when properly defined, satisfy the Wheeler–DeWitt equation up to the K_0 term in the action [39,44]. We have seen that the initial conditions in the minisuperspace action are already at the classical level an issue where the $(3+1)$ split dynamics becomes degenerate and one has to resort to the four-dimensional geometrical picture. We therefore feel justified to resort to the four-dimensional geometrical picture also at the level of the path integral, in the form of the Wheeler–DeWitt equation, to discuss the initial conditions of the integral. This reasoning is admittedly far from elegant, and, worse still, it also contains a degree of arbitrariness. One might therefore regard just the self-consistency of the results obtained as the best justification of our method of choosing the initial conditions at the level of the path integral.

Although the thermodynamical properties of our partition function far below the Planck regime were found to agree closely with those of the partition function obtained by Whiting and York, the densities-of-states were drastically different for energies above the classical threshold for positive temperatures. On the one hand this is mathematically understandable, since the inverse Laplace transform which gives the density-of-states from the partition function is sensitive to the behaviour of the partition function not only at real temperatures much below Planck scale, but also at complex values of the temperature. Another example of this kind of behaviour is that if one attempts to compute the density-of-states using the approximate formula (5.1), one finds a result which is correct (vanishing) for $E \leqslant 0$ and semiclassically correct for $0 \leqslant E \leqslant r_0$, but becomes increasingly inaccurate at large energies and only falls off as $E^{-1/2}$ at $E \to \infty$. On the other hand, it is not clear what one should understand as the implications of this difference in the two respective methods of evaluating the partition function. An argument for preferring the method of this paper might be, in addition to the relation to the Wheeler–DeWitt equation, the fact that our density-of-states corresponds more closely to the semiclassical analysis of the density-of-states given in [4].

It would be straightforward to generalize the method of this paper to incorporate a non-vanishing cosmological constant Λ. The only difference in (3.9) would be that the argument of I_0 would be multiplied by an additional factor [12]

$$\left[1-(\Lambda/3)\left(r_0^2+r_0r_+ + r_+^2\right)\right]^{1/2}. \tag{6.1}$$

Also the density-of-states could be computed in essentially the same manner. It appears however not presently understood whether one should expect the resulting expressions to have a thermodynamical interpretation.

In this paper we first computed a partition function from a path integral, and only after that computed the density-of-states from the partition function by an inverse Laplace transform. It might be considered of interest to attempt a computation of the density-of-states directly from a path integral [45]. More generally, it might be of interest to consider ensembles where one does not fix the area of the box but its conjugate, a pressure-like quantity [8]. Although the resulting amplitudes are expected to be related to each other by Fourier–Laplace type transformations, it is not clear that one will be able to derive satisfactory path integral representations for all of them once a path integral representation for one is given. In investigating this, one would at least need to show, in detail, how to take the integral transforms under the path integral. One potentially severe complication here is that the contours of integration in the path integrals may be complex in a rather involved way, as was the case in this paper. This is essentially the same issue which was mentioned previously in this section in the context of the different classically equivalent initial data sets in the path integral.

Finally, in all of this paper we have taken the manifold inside the four-dimensional Euclideanized box to be $\bar{D} \times S^2$, for which the classical solutions to the boundary value problem are sections of the Euclidean Schwarzschild solution. Another manifold of interest is $\bar{B}^3 \times S^1$, where $\bar{B}^3$ is the closed three-dimensional ball. In this case the classical solution is Euclidean flat space with a periodic time coordinate. The two manifolds have been referred to as the black hole topological sector and the hot flat space topological sector, respectively [3–5, 7]. If a total partition function is taken to consist of the black hole sector contribution considered in this paper and a flat space sector contribution, with coefficients of order unity, a semiclassical estimate shows that the flat space sector and the black hole sector dominate respectively for low and high temperatures. This has been interpreted as semiclassical evidence of topology change inside the box as the boundary temperature is made to change [3, 5, 7]. Whilst it might be possible to apply methods similar to ours to a minisuperspace path integral for the flat space sector contribution, our method does not appear to provide new arguments for fixing the relative weights of the two sectors. Our work does therefore not appear to alter current insight on the possibility of a topological phase transition, or on the stability of flat space against black hole nucleation.

It is clear that a more complete treatment of all the gravitational degrees of freedom would involve dealing with the non-spherical modes which have been neglected in this paper, both propagating and non-propagating. Even though many of the issues remain unresolved in connection with a complete formulation for the path integral for these degrees of freedom, it is nevertheless reasonable to expect that when they are all integrated out there will remain an analogue of the r_+ integral which has here arisen entirely in the context of spherically symmetric geometries. It is particularly noteworthy that, in choosing an appropriate contour, we found it so helpful to be able to refer to a physical argument about the thermodynamic stability as evinced by a positive heat capacity for the classical solution which dominated the partition function. We expect that most of the questions which we have addressed in this paper will continue to exist, and that the work here might present a basis for methods of dealing with them in the future.

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