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Finite temperature and boundary effects in static space-times

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Abstract. Expressions are derived for the free energy of a massless scalar gas confined to a spatial cavity in a static space-time at a finite temperature. A high temperature expansion is presented in terms of the Minakshisundaram coefficients. This gives curvature and boundary corrections to the Planckian form. The regularisation used is the zeta function one, and yields a finite total internal energy. However, it is known that the local energy density diverges in a non-integrable way as the boundary is approached. A 'surface energy' is suggested to reconcile these two facts. Explicit expressions for the total energy inside two infinite rectangular waveguides are obtained.

1. Introduction

The system under investigation in the present work is a quantum field at finite temperature in a static space-time that may have boundaries. Since a number of review articles have recently appeared (DeWitt 1975, Isham 1977, Davies 1976) it is unnecessary to repeat the motivation for studying field theory in curved space-time. In an earlier work (Dowker and Critchley 1977a) we discussed the case of a scalar field in an Einstein universe and derived the effective Lagrangian and stress-energy tensor at a finite temperature. This case, while it admits of an explicit solution, is a rather restricted one and we would like to have more general expressions.

One of the things we will derive is the correction to the Planck distribution, at high temperatures, due to the curvature and boundaries. The effects of boundaries are well known in various topics and have been usefully summarised in the review by Baltes and Hilf (1976). The curvature effects do not seem to be so generally familiar.

2. Basic formalism

To avoid technical difficulties we shall consider only the conformally coupled real scalar field, ϕ , which satisfies

$$(\Box - \frac{1}{6}R)\phi = 0; \qquad \Box \phi \equiv \phi_{\parallel \mu}{}^{\mu} = \nabla^{\mu}\nabla_{\mu}\phi.$$
(1)

An action for this field is

$$S = -\frac{1}{2}(\phi | G^{-1} | \phi)$$
⁽²⁾

where we use a formal, covariant space-time matrix notation (DeWitt 1975, 1965).

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Thus

$$\phi(x) = (x|\phi),$$

and the orthogonality and completeness relations read

$$(x|x') = \delta(x, x') = g^{-1/4}(x)\delta(x - x')g^{-1/4}(x')$$

and

$$\int d^4x |x\rangle g^{1/2}(x) = 1; \qquad g \equiv -\det g_{\mu\nu}.$$

In (2), G^{-1} is the operator in (1) and its coordinate space representation is

$$(x|G^{-1}|x') = (\Box - \frac{1}{6}R)\delta(x, x').$$

The finite-temperature effective action is introduced in the same way as at zero temperature (e.g. DeWitt 1965, 1975). Firstly from (2) we have for a small change in the parameters specifying the system

$$\delta S = -\frac{1}{2}(\phi | \delta G^{-1} | \phi). \tag{3}$$

Next the $|\phi\rangle$ are interpreted as quantum operators and the thermal average of (3) taken, which yields

$$\langle \delta \hat{S} \rangle = -\frac{1}{2} \langle (\hat{\phi} | \delta G^{-1} | \hat{\phi}) \rangle \tag{4}$$

where the angular brackets signify the usual statistical averaging over a canonical ensemble,

$$\langle \hat{A} \rangle \equiv \mathrm{Tr}(\mathrm{e}^{-\beta_0 \hat{H}} \hat{A}) / \mathrm{Tr}(\mathrm{e}^{-\beta_0 \hat{H}}).$$
(5)

The trace in this formula signifies a trace in the quantum field Hilbert space, and \hat{H} is the second quantised field Hamiltonian whose exact form will be given later.

It is necessary to state now that in order that conventional concepts about thermal averaging be still valid the space-time, \mathcal{M} , must be restricted to be static. Then \hat{H} is time independent.

The next step is to define the finite-temperature (Feynman) Green function $G_{\beta_0}(x, x')$ as (Dowker and Critchley 1977a, Gibbons and Perry 1977, Dolan and Jackiw 1974, Bernard 1974, Martin and Schwinger 1959)

$$G_{\beta_0}(x, x') = i\langle T\{(x|\hat{\phi})(\hat{\phi}|x')\}\rangle,\tag{6}$$

 $T\{\ldots\}$ standing for the time ordered product with respect to the static time coordinate t in the coordinate system,

$$ds^{2} = g_{00}(\mathbf{x}) dt^{2} + g_{ij}(\mathbf{x}) dx^{i} dx^{i}; \qquad (\det g_{ij} < 0, \mathbf{x} = \{x^{i}\}).$$
(7)

Then (4) is re-written, as in the zero-temperature case,

$$\delta W_{\beta_0}^{(1)} = \langle \delta \hat{S} \rangle = \frac{1}{2} i \operatorname{tr}(G_{\beta_0} \delta G^{-1}), \tag{8}$$

the trace operation this time being a covariant space-time integration,

$$\operatorname{tr} \boldsymbol{A} = \int \mathrm{d}^4 x \, g^{1/2}(x |\boldsymbol{A}| x).$$

It is important to remember that G_{β_0} satisfies the same equation as G_{∞} , the zero-temperature Green function, i.e. the usual one G (Dolan and Jackiw 1974,

Martin and Schwinger 1959). Thus,

$$(\Box - \frac{1}{6}R)G_{\beta_0}(x, x') = \delta(x, x')$$

or, formally, in operator notation

$$G^{-1}G_{\beta_0}=1.$$

Then equation (8) reads

$$\delta W_{\beta_0}^{(1)} = \frac{1}{2} i \operatorname{tr}(G_{\beta_0} \, \delta G_{\beta_0}^{-1}) = -\frac{1}{2} i \delta \operatorname{tr}(\ln G_{\beta_0}) = -\frac{1}{2} i \delta \ln \operatorname{Det} G_{\beta_0}. \tag{9}$$

We thus arrive at the formally divergent expression for the finite-temperature oneloop effective action

$$W_{\beta_0}^{(1)} = -\frac{1}{2}i \operatorname{tr}(\ln G_{\beta_0}) = -\frac{1}{2}i \ln \operatorname{Det} G_{\beta_0}$$
(10)

plus, possibly, a metric-independent constant of integration which we ignore.

Before going on to regularise $W_{\beta_0}^{(1)}$ it is convenient to use the static nature of the system to introduce the Lagrangian rather than the action as the important invariant.

Thus write for the effective action (the same is true for the classical action S)

$$W_{\beta_0}^{(1)} = \int \mathrm{d}t \, L_{\beta_0}^{(1)}$$

where the Lagrangian L is time independent. The thermally averaged stress-energy tensor $\langle \hat{T}^{\mu\nu} \rangle$ is now determined by functionally differentiating $L_{\beta_0}^{(1)}$ rather than $W_{\beta_0}^{(1)}$,

$$\langle \hat{T}_{00} \rangle = 2g^{-1/2} \,\delta L^{(1)}_{\beta_0} / \delta g^{00}(\mathbf{x}), \qquad \langle \hat{T}_{ij} \rangle = 2g^{-1/2} \,\delta L^{(1)}_{\beta_0} / \delta g^{ij}(\mathbf{x}) \tag{11}$$

with

$$\langle \hat{T}_{i0} \rangle = 0. \tag{12}$$

In a more general space-time it would not be possible to get away with differentiating with respect to the metric functions in some particular coordinate system. For example if g_{i0} were zero one could not conclude that $\langle \hat{T}_{i0} \rangle$ would also vanish in this frame (R_{i0} might not be zero) so that, if one wanted these components, a more general metric would have to be used. However in a static space-time there are no geometrical tensors that have one spatial index and one temporal, so that (12) must be true and then (11) is sufficient. It is assumed of course that the entire theory is generally covariant.

From (10) the expression for the effective Lagrangian is

$$L_{\beta_0}^{(1)} = -\frac{1}{2}i \operatorname{tr}_3(\ln G_{\beta_0}), \tag{13}$$

where tr_3 stands for an integration over the spatial section of \mathcal{M} ,

$$\operatorname{tr}_{3} \boldsymbol{A} \equiv \int \mathrm{d}\boldsymbol{x} \, g^{1/2}(\boldsymbol{x}, t | \boldsymbol{A} | \boldsymbol{x}, t).$$

Incidentally if the imaginary time representation had been employed (cf Bernard 1974, Hawking 1977) we could have retained the (imaginary) time integration and divided by its range, β_0 to give the Lagrangian.

Turning now to the regularisation of (13) our method of making $L_{\beta_0}^{(1)}$ finite is that introduced in Dowker and Critchley (1976a) as zeta function regularisation. The expressions can be most rapidly obtained as follows.

In the expression $tr_3(G_{\beta_0} \delta G_{\beta_0}^{-1})$ occurring in the formula for $\delta L_{\beta_0}^{(1)}$, corresponding to (9), the factor of G_{β_0} coming from (6) is replaced by the formal power $G_{\beta_0}^s$. If Re s > 2 everything converges and the physical quantity is obtained by continuing s into the complex plane and down to s = 1. The divergence is then neatly displayed as a pole in s at s = 1.

Performing this sequence of operations yields,

$$\operatorname{tr}_{3}(G_{\beta_{0}} \,\delta G_{\beta_{0}}^{-1}) \to \operatorname{tr}_{3}(G_{\beta_{0}}^{s} \,\delta G_{\beta_{0}}^{-1}) = -\frac{1}{s-1} \delta \,\operatorname{tr}_{3}(G_{\beta_{0}}^{s-1})$$

whence

$$L_{\beta_0}^{(s)} = -\frac{i}{2} \frac{1}{s-1} \operatorname{tr}_3 \zeta(s-1, \beta_0), \tag{14}$$

where the continuation of $G_{\beta_0}^s$ to the whole s plane produces the finite-temperature zeta function, $\zeta(s, \beta_0)$ on the space-time.

Setting s equal to one in this continued expression produces the regularised one-loop effective Lagrangian,

$$L_{\beta_{0}}^{(1)} = \lim_{s \to 1} L_{\beta_{0}}^{(s)} = -\frac{i}{2} \left(\frac{\operatorname{tr}_{3} \zeta(0, \beta_{0})}{s - 1} + \operatorname{tr}_{3} \zeta'(0, \beta_{0}) \right).$$
(15)

The analysis of expressions (14) and (15) will continue in §4.

3. Quantisation in static space-times and the optical metric

In static space-times the quantisation procedure more or less parallels that in Minkowski space-time. It has been given, together with a discussion of the inherent non-uniqueness by Fulling (1973) and we shall simply use his results (see also Gibbons and Perry 1977, Kramer and Lotze 1974, Unruh 1974a, b, Ashtekar and Magnon 1975, Dowker and Critchley 1977a).

In the static coordinate frame (7) the mode decomposition of the field $\phi(x)$ is

$$\hat{\phi} = \sum_{k} (2\omega_k)^{-1} (a_k e^{-i\omega_k t} \phi_k + a_k^{\dagger} e^{i\omega_k t} \phi_k^{\ast})$$
$$= \sum_{k} g_{00}^{-1/2} (2\omega_k)^{-1} (a_k e^{-i\omega_k t} \bar{\phi}_k + a_k^{\dagger} e^{i\omega_k t} \bar{\phi}_k^{\ast})$$

where the mode functions ϕ_k , satisfy the elliptic equation

 $(\bar{\Delta}_2 + \bar{g}^{ij}\partial_i \ln g_{00}\partial_j + \frac{1}{6}\bar{R} + \frac{1}{2}\bar{\Delta}_2 \ln g_{00} + \frac{1}{4}\bar{g}^{ij}\partial_i \ln g_{00}\partial_j \ln g_{00})\phi_k = \omega_k^2\phi_{k'}$

or, equivalently,

$$(\bar{\Delta}_2 + \frac{1}{6}\bar{R})\bar{\phi}_k = \omega_k^2 \bar{\phi}_k \tag{16}$$

with

$$\bar{\phi}_k = g_{00}^{1/2} \phi_k.$$

In these equations the barred quantities are calculated using the 'optical metric', $\bar{g}_{\mu\nu} \equiv g_{\mu\nu}/g_{00}$ ($\bar{g}^{\mu\nu} = g^{\mu\nu}g_{00}$) (see Gibbons and Perry 1977) and Δ_2 is the Laplace-Beltrami operator on the three-space. From (16) we note the important fact that the eigenvalues ω_k are conformally invariant, because two conformally related metrics have the same optical metric.

The field Hamiltonian H is given by

$$H=\int \mathrm{d}\boldsymbol{x}\,g^{1/2}T_0^{0},$$

where the energy density T_0^{0} is given by

$$T_0^{0} = 2g^{-1/2}g^{00}\frac{\delta L}{\delta g^{00}},$$

with $S = \int L dt$, given by (2). Then the mode decomposition gives the quantum field Hamiltonian \hat{H} as

$$\hat{H} = \frac{1}{2} \sum_{k} \omega_k \{a_k, a_k^{\dagger}\} = \sum_{k} \omega_k (\hat{N}_k + \delta_{k,k}).$$

$$(17)$$

In this derivation we must use the fact that the mode functions $\bar{\phi}_k$ are normalised with respect to the weight provided by the optical metric $\bar{g}_{\mu\nu}$.

The statistical mechanics of the system can be developed by constructing the partition function Z:

$$Z = \mathrm{Tr}(\mathrm{e}^{-\beta_0 H}) \tag{18}$$

using the \hat{H} of (17) and the properties of the eigenvalues ω_k . Rather than Z it is often more convenient to use the free energy F:

$$F = -\beta_0^{-1} \ln Z = E - TS; \quad \text{or} \quad E = \frac{\partial(\beta_0 F)}{\partial \beta_0}$$
(19)

where S is the entropy and E the internal energy,

 $E = \langle \hat{H} \rangle.$

A variational expression for E can be found from (11) by re-scaling g_{00} by a constant factor, $g_{00} \rightarrow \alpha^2 g_{00}$. It is easy to show that

$$E = -\frac{d}{d\alpha} L^{(1)}_{\beta_0}[\alpha^2 g_{00}]\Big|_{\alpha=1}.$$
 (20)

In fact it appears we can go further and relate the free energy to the effective Lagrangian. To do this we use equation (14) in order to see how $L_{\beta_0}^{(s)}$ changes when g_{00} is re-scaled. First, however, a closer inspection of the meaning of the 'power' $G_{\beta_0}^s$ is necessary.

4. The free energy and effective Lagrangian

Generally speaking a precise meaning can be given to the power A^s only if A is an elliptic operator. In the present case, for G^{-1} , this can be achieved by working in the Euclideanised space-time \mathcal{M}_E obtained by the replacement $t \rightarrow it$ from \mathcal{M} . Then $G^s_{\beta_0}$ is the matrix power of G_{β_0} with all interior real time integrations restricted to the interval 0 to $i\beta_0$.

Consider the quantity $\operatorname{tr}_3(G_{\beta_0}^{s-1}) \sim \operatorname{tr}_3 \zeta(s-1, \beta_0)$ needed in (14) and re-scale $g_{00} \rightarrow \alpha^2 g_{00}$. Imagine the product of s-1 G_{β_0} 's written out. There will be s-2 space-time integrations. Concentrate on just the time integrations, each of which runs from 0 to $i\beta_0$. The factor of $g^{1/2}$ at each integration acquires a scaling of α and we may combine this with the dt to call αt , t' and obtain s-2 t' integrations running from 0 to $i\alpha\beta_0$. The Green function factors will each be like $G_{\beta_0}(\alpha^{-1}t'_i - \alpha^{-1}t'_j; \alpha^2 g_{00})$, where we have displayed dependence on $\alpha^2 g$. Now, re-scaling g_{00} is equivalent to re-scaling t so that we have the relation

$$G_{\beta_0}(\alpha^{-1}t'; \alpha^2 g_{00}) = G_{\alpha\beta_0}(t'; g_{00}).$$
(21)

Note that β_0 has been re-scaled on the right so that both sides have the same periodicity in t', namely $i\alpha\beta_0$.

Equation (21) shows that $tr_3 G^{s-1}$ scales as

$$(\mathrm{tr}_3 \ G_{\beta_0}^{s-1})[\alpha^2 g_{00}] = \alpha (\mathrm{tr}_3 \ G_{\alpha\beta_0}^{s-1})[g_{00}]$$
(22)

where the overall factor of α comes from the $g^{1/2}$ in the definition of tr₃.

If s is continued into the complex plane and (14), or (15), used we find

$$L^{(1)}_{\beta_0}[\alpha^2 g_{00}] = \alpha L^{(1)}_{\alpha\beta_0}[g_{00}]$$

and then (20) rapidly produces

$$E = -\frac{\partial}{\partial \beta_0} (\beta_0 L_{\beta_0}^{(1)}).$$
⁽²³⁾

Comparison with (19) yields the relation between the free energy and the effective Lagrangian,

$$F = -L_{\beta_0}^{(1)} + M/\beta_0 \tag{24}$$

where M is temperature independent and is, so far, undetermined apart from satisfying the condition

$$M(\alpha^2 g_{00},\ldots) = M(g_{00},\ldots).$$

The zero-temperature relation

$$F(\infty) = -L_{\infty}^{(1)}$$

is found by setting β_0 equal to infinity in (24). The zero-temperature free energy $F(\infty)$ equals the zero-temperature internal energy $E(\infty)$ which is just the vacuum average of \hat{H} . Thus we have the useful relation

$$F(\infty) = E(\infty) = -L_{\infty}^{(1)}.$$
(25)

Although our main interest is with a general static metric having a non-constant g_{00} it is useful at this stage to consider the ultrastatic case, in Fulling's (1973) terminology, for which g_{00} is constant, say one. Since the optical metric is ultrastatic we can use the barred notation, and refer to the ultrastatic metric as the optical metric.

In the optical metric \overline{M} , in equation (24), is zero. This can be shown in several ways. We can begin again and construct both F and $-L_{\infty}^{(1)}$ to show they are equal. Alternatively we can note that at low temperature, $\beta_0 \rightarrow \infty$, both F and $L_{\beta_0}^{(1)}$ vanish exponentially fast. Hence there can be no β_0^{-1} term in (24).

To see this in more detail we proceed to give some explicit constructions. Firstly we must now say that in this paper the time variable t is allowed to run from $-\infty$ to $+\infty$ and that the spatial section of \mathcal{M} , denoted by \mathcal{M}_3 , is compact with a boundary, $\partial \mathcal{M}_3$. For simplicity (\mathcal{M}, g) is denoted by \mathcal{M} while the optical manifold (\mathcal{M}, \bar{g}) is written as $\bar{\mathcal{M}}$, and similarly for the spatial section and boundary. $\bar{\mathcal{M}}$ is the direct product of the time axis T and the spatial section $\bar{\mathcal{M}}_3$.

In Dowker and Critchley (1976a) the zeta function was related to the proper time quantum mechanical propagator, K, and a similar expression can be employed in the present case. We write the Mellin transform

$$(x|\zeta(s,\beta_0)|x') = \frac{e^{i\pi s/2}}{\Gamma(s)} \int_0^\infty d\tau \, \tau^{s-1} K_{\beta_0}(x,x',\tau)$$
(26)

where $K_{\beta_0}(x, x', \tau)$ satisfies the Schrödinger equation

$$\left(i\frac{\partial}{\partial\tau}-\Box+\frac{1}{6}R\right)K_{\beta_0}(x,x',\tau)=ig^{-1/2}\delta(x-x')\delta(\tau)$$

and has period β_0 in imaginary time.

It is shown in Dowker and Critchley (1977a) and Dowker (1977) that K_{β_0} , and also G_{β_0} , can be expressed as image sums of zero-temperature quantities,

$$K_{\beta_0}(x, x', \tau) = \sum_{m=-\infty}^{\infty} K_{\infty}(x, x' - \mathrm{i}m\lambda\beta_0, \tau)$$
(27)

where λ is the time-like unit vector (1, 0, 0, 0).

In the optical manifold, time is completely separated from space and the propagator \bar{K} factors so that if (27) is used we find for $\bar{\text{tr}}_3 \tilde{\zeta}(s, \beta_0)$, which is needed in equation (15) for $\bar{L}_{\beta_0}^{(1)}$,

$$\begin{aligned} \widetilde{\mathrm{tr}}_{3}\,\,\widetilde{\boldsymbol{\zeta}}(s,\,\beta_{0}) &= \mathrm{i}\,\frac{\mathrm{e}^{\mathrm{i}\,\pi s/2}}{\Gamma(s)} \int \mathrm{d}\tau \frac{\tau^{s-1}}{(4\,\pi\mathrm{i}\,\tau)^{1/2}} \sum_{m} \mathrm{e}^{\mathrm{i}\,m^{2}\beta_{0}^{2}/4\tau} \overline{K}_{3}(\tau) \end{aligned} \tag{28a} \\ &= \mathrm{i}\,\frac{\mathrm{e}^{\mathrm{i}\,\pi s/2}}{\Gamma(s)} \int \mathrm{d}\tau \frac{\tau^{s-1}}{(4\,\pi\mathrm{i}\,\tau)^{1/2}} \theta_{3}\Big(0,\frac{\beta_{0}^{2}}{4\,\pi\tau}\Big) \overline{K}_{3}(\tau) \\ &= \frac{\mathrm{i}}{\beta_{0}}\,\frac{\mathrm{e}^{\mathrm{i}\,\pi s/2}}{\Gamma(s)} \int_{0}^{\infty} \mathrm{d}\tau\,\tau^{s-1} \theta_{3}\Big(0,-\frac{4\,\pi\tau}{\beta_{0}^{2}}\Big) \overline{K}_{3}(\tau) \\ &= \frac{\mathrm{i}}{\beta_{0}}\,\frac{\mathrm{e}^{\mathrm{i}\,\pi s/2}}{\Gamma(s)} \int_{0}^{\infty} \mathrm{d}\tau\,\tau^{s-1} \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\,4\,\pi^{2}n^{2}\tau/\beta_{0}^{2}} \overline{K}_{3}(\tau) \end{aligned} \tag{28b}$$

where

$$\bar{K}_3(\tau) = \overline{\mathrm{tr}}_3 \, K_3(\tau) \equiv \int \mathrm{d} x \, \tilde{g}^{1/2} \bar{K}_3(x, x, \tau).$$

 $\tilde{K}_3(x, x', \tau)$ is the propagator on the spatial manifold $\tilde{\mathcal{M}}_3$, and satisfies the equation:

$$\left(\frac{\partial}{\partial \tau}-\bar{\Delta}_2-\frac{1}{6}\bar{R}\right)\bar{K}_3(\boldsymbol{x},\boldsymbol{x}',\tau)=\mathrm{i}\bar{g}^{-1/2}\delta(\boldsymbol{x}-\boldsymbol{x}')\delta(\tau),$$

subject to the boundary conditions appropriate to $\tilde{\mathcal{M}}_3$. For example if $\partial \tilde{\mathcal{M}}_3 \neq \emptyset$ one would typically make $\bar{K}_3(\mathbf{x}, \mathbf{x}', \tau)$ vanish if either \mathbf{x} or $\mathbf{x}' \in \partial \tilde{\mathcal{M}}_3$. Perhaps it is worth-while interjecting some general remarks on boundary conditions.

These can be imposed when solving the mode equations (16) and we shall consider only Dirichlet or Neumann (D or N) conditions and apply them to the $\overline{\phi}$ functions. This is more convenient than using the ϕ because it makes the analysis in the optical metric relevant for the general case to which it is conformally related. These boundary conditions mean that there is no $\overline{\phi}$, or ϕ , flux across ∂M_3 .

In terms of the eigenfunctions $\bar{\phi}_k$ and eigenvalues ω_k , \bar{K}_3 can be written

$$\bar{\boldsymbol{K}}_{3} = \sum_{k} e^{-i\omega_{k}^{2}\tau} |\bar{\boldsymbol{\phi}}_{k}\rangle (\bar{\boldsymbol{\phi}}_{k}|.$$
⁽²⁹⁾

Substituted into (28b), the form (29) yields for the integrated zeta function the expression used by, e.g., Hawking (1977) in a special case (see also Gibbons 1977):

$$\overline{\mathrm{tr}}_{3}\,\overline{\boldsymbol{\zeta}}(s,\,\beta_{0}) = \frac{\mathrm{i}}{\beta_{0}}\sum_{n,\omega_{k}}\frac{d_{k}}{[\omega_{k}^{2} + (4n^{2}\pi^{2}/\beta_{0}^{2})]^{s}}.$$
(30)

 d_k is the degeneracy of the kth mode. If one knows the properties of the modes explicitly it may be possible to relate this expression to already defined zeta functions. In the Einstein universe, for example, this can be done (Dowker and Al'taie 1978).

On the other hand if (29) is substituted into (28*a*) and the m = 0 term, which is just the zero-temperature expression, separated off we find for $\overline{L}_{\beta_0}^{(1)}$ a familiar statistical mechanical sum-over-states form, after summing over m,

$$\bar{L}_{\beta_0}^{(1)} = -\frac{i}{2} \lim_{s \to 1} \frac{\bar{tr}_3 \, \bar{\zeta}(s-1, \beta_0)}{s-1} = -\beta_0^{-1} \sum_{\omega_k} d_k \, \ln(1 - e^{-\beta_0 \omega_k}) + \bar{L}_{\infty}^{(1)}. \tag{31}$$

Equations (17), (18), (19), (25), and (31) allow us to identify \overline{F} and $-\overline{L}_{\beta_0}^{(1)}$, as mentioned before

Expression (31) is the one suitable for low temperatures, and it can be seen that, if the ω_k are discrete, as they are if \mathcal{M}_3 is compact, then \overline{F} tends to $\overline{F}(\infty)$ exponentially fast as $\beta_0 \rightarrow \infty$. However, if the system becomes non-compact, to give a continuous eigenvalue running from 0 to ∞ , there will be a polynomial behaviour at small temperatures. For example in the parallel-plate geometry there is an extra β_0^{-3} term, while for the cylinder we find β_0^{-2} (see equation (59)).

Equation (31) also shows that the infinities reside entirely in the zero-temperature part, $\bar{L}_{\infty}^{(1)}$. This is generally true. If the behaviour near $\tau = 0$ of the integrand in the expression for tr₃ $\zeta(s, \beta_0)$ obtained from (26) and (27),

$$\operatorname{tr}_{3} \boldsymbol{\zeta}(s,\beta_{0}) = \sum_{m} \frac{\mathrm{e}^{\mathrm{i}\pi s/2}}{\Gamma(s)} \int_{0}^{\infty} \mathrm{d}\tau \, \tau^{s-1} \int \mathrm{d}\boldsymbol{x} \, g^{1/2} K_{\infty}(x,\,x-\mathrm{i}m\lambda\beta_{0},\,\tau), \tag{32}$$

is investigated, it can be seen that only for the m = 0 term (the zero-temperature expression) do we need the condition s > 2 for convergence. In the other terms $(m \neq 0)$ the K_{∞} factor provides all the convergence needed since it goes to zero exponentially fast. Thus, if we set s = 0, the pole in $\Gamma(s)$ will kill every term except the m = 0 one. Equation (15) can then be re-written:

$$L_{\beta_0}^{(1)} = -\frac{i}{2} \left(\frac{\mathrm{tr}_3 \, \boldsymbol{\zeta}(0, \infty)}{s - 1} + \mathrm{tr}_3 \, \boldsymbol{\zeta}'(0, \beta_0) \right) \tag{33}$$

showing clearly that the divergence is temperature independent. The renormalisation of the Lagrangian is thus the zero-temperature renormalisation.

Returning to the optical metric and equation (31), if the space-time in which we are interested really is ultrastatic $(g_{00} = 1)$ the renormalised free energy would be obtained as the negative of the renormalised effective Lagrangian which is obtained from the $\bar{L}_{\beta_0}^{(1)}$ of (31) by replacing $\bar{L}_{\infty}^{(1)}$ by its renormalised expression, in accordance with the previous remarks.

Without, at this stage, entering into any details, the renormalised $L_{\infty}^{(1)}$ is found by dropping the pole term in (33), for $\beta_0 = \infty$, and we can write

$$\bar{F}_{ren} = \lim_{s \to 1} \left(\bar{F}^{(s)} - \frac{i}{2} \frac{\bar{t}r_3 \, \bar{\xi}(0, \infty)}{s - 1} \right)$$
(34)

where $\bar{F}^{(s)} = -\bar{L}^{(s)}$.

In order to obtain an expression suitable for high temperatures it is necessary to use the asymptotic expansion of $\bar{K}_3(\tau)$ in powers of τ ,

$$\bar{K}_{3}(\tau) = (4\pi i\tau)^{-3/2} \sum_{l=0,\frac{1}{2},1,\frac{3}{2},\dots} \bar{c}_{l}(i\tau)^{l} + \text{ES}$$
(35)

where Es stands for terms which vanish exponentially fast as τ tends to zero. The \bar{c}_l are Minakshisundaram coefficients (Minakshisundaram and Pleijel 1949) modified by the presence of the boundary. They may be written as (Greiner 1971, Gilkey 1975c) a volume part plus a boundary part,

$$\bar{c}_{l} = \int_{\bar{\mathcal{A}}_{3}} \mathrm{d}\boldsymbol{x} \, \bar{\boldsymbol{g}}^{1/2} \bar{a}_{l}(\boldsymbol{x}, \boldsymbol{x}) + \int_{\partial \bar{\mathcal{A}}_{3}} \mathrm{d}\tilde{\sigma} \, \bar{b}_{l}(\boldsymbol{x})
\equiv \bar{a}_{l} + \bar{b}_{l}.$$
(36)

The $\bar{a}_l(\mathbf{x}, \mathbf{x}')$ are the Minakshisundaram coefficients for the case $\partial \bar{\mathcal{M}}_3 = \emptyset$ if *l* is integral and vanish if *l* is half integral. The coincidence limits $\bar{a}_l(\mathbf{x}, \mathbf{x})$ are given by local expressions in terms of the metric on $\bar{\mathcal{M}}_3$. Expressions for the \bar{a}_1 , \bar{a}_2 and \bar{a}_3 coefficients have been given (DeWitt 1965, Sakai 1971). The $\tilde{b}_l(\mathbf{x})$ depend on the induced metric and extrinsic curvature of $\partial \bar{\mathcal{M}}_3$. Further comments will be found later.

It is clear that this form of $\bar{K}_3(\tau)$ is useful only for small τ or for cases where convergence as τ becomes large can be ensured as, for example, in the case of a massive field treated by Dowker and Critchley (1976a) or as in equation (28b) for all terms in the sum except the n = 0 one. In this case therefore we will have from (26), (28b) and (35) an asymptotic expansion for the zeta function in inverse powers of the temperature $1/\beta_0$, if we separate off the n = 0 term,

C stands for the contribution of the ES terms in (35) which are significant if τ is not small. As β_0 increases, the upper τ integration range becomes more important and C is then not negligible. Roughly speaking the asymptotic expansion is valid if $\beta_0^{-1}D \ge 1$, where D is the typical dimension or size of \overline{M}_3 , From now on we drop C.

 $\bar{\zeta}_3(s,\infty)$ is the ordinary (zero-temperature) zeta function on the spatial section, $\bar{\mathcal{M}}_3$, and $\zeta_{\mathbf{R}}(s)$ is the Riemann zeta function. The relation between (37*a*) and (37*b*) follows from the functional relation satisfied by $\zeta_{\mathbf{R}}(s)$.

Equation (14) with (37) now allows us to find the expansion for the free energy \vec{F} :

$$\bar{F} = \lim_{s \to 1} \bar{F}^{(s)} = -\frac{\pi^2}{90} \frac{\bar{c}_0}{\beta_0^4} - \frac{\zeta_R(3)}{4\pi^{3/2}} \frac{\bar{c}_{1/2}}{\beta_0^3} - \frac{1}{24} \frac{\bar{c}_1}{\beta_0^2} - \overline{\mathrm{tr}}_3 \bar{\zeta}_3^{\prime}(0,\infty) \frac{1}{2\beta_0} + \frac{1}{2\beta_0(s-1)} \left(\frac{1}{8\pi^{3/2}} \bar{c}_{3/2} - \overline{\mathrm{tr}}_3 \bar{\zeta}_3(0,\infty) \right) + \frac{\bar{c}_{3/2}}{8\pi^{3/2}} \frac{1}{\beta_0} \ln \beta_0 - \frac{\bar{c}_2}{16\pi^2} \left[\ln \left(\frac{\beta_0}{4\pi} \right) + \gamma \right] - \frac{1}{32\pi^2} \frac{\bar{c}_2}{s-1} - \frac{\pi^{3/2}}{16} \sum_{l=5/2}^{\infty} \bar{c}_l \Gamma(l-\frac{3}{2}) \times \zeta_R(2l-3)\pi^{-2l} \left(\frac{\beta_0^2}{4} \right)^{l-2},$$
(38)

where $\gamma \equiv -\psi(1)$. From this expression we must subtract the pole term, as in (34), to get the renormalised free energy \overline{F}_{ren} . To show that there are no pole terms remaining in \overline{F}_{ren} we have recourse to a result of zeta function theory (e.g. Minakshisundaram and Pleijel 1949) that in *d* dimensions the integrated zeta function tr_d $\zeta_d(s, \infty)$ evaluated at s = 0 is proportional to the $c_{d/2}$ coefficient in the expansion of tr_d $K_d(\tau)$,

$$\operatorname{tr}_{d} \zeta_{d}(0,\infty) = (4\pi)^{-d/2} c_{d/2}.$$
(39)

Applied firstly to the spatial sections, $\bar{\mathcal{M}}_3$, (39) gives

$$\overline{\mathrm{tr}}_{3}\,\overline{\zeta}_{3}(0,\,\infty) = \frac{1}{8}\pi^{-3/2}\overline{c}_{3/2}$$

which shows that the $\bar{c}_{3/2}$ pole cancels the $\bar{\zeta}_3(0, \infty)$ term in (38). When applied to the space-time, $\bar{\mathcal{M}}$, for which d = 4, we can remove the time integration in the tr₄ to give tr₃ since the integrands are time independent. Thus

$$\overline{\mathrm{tr}}_{3}\,\overline{\boldsymbol{\zeta}}(0,\,\infty) = \mathrm{i}(16\,\pi^{2})^{-1}\,\overline{c}_{2},\tag{40}$$

where the factor of i comes from the continuation from the Euclideanised space $\overline{\mathcal{M}}_{E}$. This result shows that the subtraction (34) cancels the \overline{c}_2 pole in (38) and we finally arrive at the 'renormalised' free energy (equivalently, the negative of the effective Lagrangian),

$$\bar{F}_{ren} = -\frac{\pi^2}{90} \frac{\bar{c}_0}{\beta_0^4} - \frac{\zeta_R(3)}{4\pi^{3/2}} \frac{\bar{c}_{1/2}}{\beta_0^3} - \frac{1}{24} \frac{\bar{c}_1}{\beta_0^2} - \bar{tr}_3 \bar{\zeta}'_3(0,\infty) \frac{1}{2\beta_0} + \frac{\bar{c}_{3/2}}{8\pi^{3/2}} \frac{1}{\beta_0} \ln \beta_0 - \frac{\bar{c}_2}{16\pi^2} \Big[\ln \Big(\frac{\beta_0}{4\pi}\Big) + \gamma \Big] - \frac{\pi^{3/2}}{16} \sum_{l=5/2}^{\infty} \bar{c}_l \Gamma(l - \frac{3}{2}) \zeta_R(2l - 3) \pi^{-2l} \Big(\frac{\beta_0^2}{4}\Big)^{l-2}.$$
(41)

For completeness we give the expansions for the internal energy \tilde{E}_{ren} and entropy \bar{S}_{ren} which follow from (41):

$$\bar{E}_{\rm ren} = \frac{\pi^2}{30} \frac{\bar{c}_0}{\beta_0^4} + \frac{\zeta_{\rm R}(3)}{2\pi^{3/2}} \frac{\bar{c}_{1/2}}{\beta_0^3} + \frac{\bar{c}_1}{24\beta_0^2} + \frac{\bar{c}_{3/2}}{8\pi^{3/2}\beta_0} - \frac{\bar{c}_2}{16\pi^2} \Big[\ln\Big(\frac{\beta_0}{4\pi}\Big) + \gamma + 1 \Big] \\ - \frac{\pi^{3/2}}{8} \sum_{l=5/2}^{\infty} \bar{c}_l \Gamma(l - \frac{1}{2}) \zeta_{\rm R}(2l - 3) \pi^{-2l} \Big(\frac{\beta_0^2}{4}\Big)^{l-2}$$
(42*a*)

$$\bar{S}_{\rm ren} = \frac{2\pi^2}{45} \frac{\bar{c}_0}{\beta_0^3} + \frac{3\zeta_{\rm R}(3)}{4\pi^{3/2}} \frac{\bar{c}_{1/2}}{\beta_0^2} + \frac{\bar{c}_1}{12\beta_0} + \frac{1}{2} \overline{\rm tr}_3 \, \bar{\zeta}_3'(0,\infty) - \frac{\bar{c}_{3/2}}{8\pi^{3/2}} (1 - \ln\beta_0) \\ - \frac{\bar{c}_2}{16\pi^2} \beta_0 - \frac{\pi^{3/2}}{4} \sum_{l=5/2}^{\infty} (l-2)\bar{c}_l \Gamma(l-\frac{3}{2}) \zeta_{\rm R}(2l-3) \pi^{-2l} \left(\frac{\beta_0^2}{4}\right)^{l-\frac{3}{2}}.$$
(42b)

The entropy is automatically finite without any subtraction.

Granted the significance of the renormalisation, and this is discussed in more detail in § 5, these expressions are of immediate value for ultrastatic space-times the simplest non-trivial example of which is probably Minkowski space-time with spatial boundaries. However our immediate aim is to extend these results to the general static metric for which $\bar{g}_{\mu\nu}$ is the optical form, and for this purpose we use a conformal transformation method.

If it were not for the infinities in the quantum field theory the statistical mechanics would be conformally invariant, determined solely by the d_k and ω_k , but infinities mean a regularisation-renormalisation process which violates the conformal invariance leading, for example, to the famous anomalies and, more pertinent to us, to different statistical mechanics.

Since it is only the zero-temperature part of the theory that has the infinities we can relate F and \overline{F} in the following manner. Equation (32) shows that the effective Lagrangian can be written as the sum of a zero-temperature part (m = 0) and a 'finite-temperature correction', i.e. the terms with $m \neq 0$. Equation (24) shows that this must be true for the free energy as well,

$$F=F(\infty)+F'.$$

The correction F' will be finite and conformally invariant so that we can equate it to its value in the optical metric,

$$F' = \overline{F}'$$
.

Then we have

$$F = F(\infty) - \bar{F}(\infty) + \bar{F} \tag{43}$$

where \overline{F} has been discussed above and for high temperature is given by (38). The advantage of this form is that we know something about $F(\infty) - \overline{F}(\infty)$ through

$$F(\infty) - \bar{F}(\infty) = \bar{L}_{\infty}^{(1)} - L_{\infty}^{(1)}.$$
(44)

The general idea is explained in Dowker and Critchley (1977b) but for completeness will be outlined here. Again for generality consider a *d*-dimensional Riemannian space and the corresponding traced zero-temperature zeta function, $\operatorname{tr}_d \zeta_d(s, g)$, where we have dropped the temperature label and replaced it by the (functional) dependence on the metric $g_{\mu\nu}$. This traced zeta function can be thought of graphically as the continuation of a 'ring' of s Green functions, G(x, x'), each x being integrated over, with a $g^{1/2}$ factor. Under the conformal transformation $g_{\mu\nu} \rightarrow \lambda^2 g_{\mu\nu}$ we know that

$$G(x, x') \rightarrow \lambda^{p}(x)G(x, x')\lambda^{p}(x')$$
 with $p = (1-d)/2$

and

$$g^{1/2} \rightarrow \lambda^{d} g^{1/2}$$

so that the only change in $\operatorname{tr}_d \zeta_d(s, g)$, $\sim \operatorname{tr} G^s$, is to introduce a factor of λ^2 at each integration point. Thus if we functionally differentiate $\operatorname{tr}_d \zeta_d(s, \lambda^2 g)$ with respect to $\lambda(x)$ we will break the ring at the integration point, x, to give a line of s Green functions and only s-1 integrations. This is the definition of the untraced (diagonal part) zeta function and we derive the theorem

$$\frac{\delta \operatorname{tr}_{d} \zeta_{d}(s, \lambda^{2}g)}{\delta \lambda(x)} = 2s\lambda(x)g^{1/2}(x)(x|\zeta_{d}(s, \lambda^{2}g)|x)$$
(45)

where the factor of s comes from the fact that there are s integration points in $tr_d \zeta_d$, each with a factor of λ^2 .

Equation (45) can be used to prove that the Minakshisundaram coefficient $c_{d/2}$, is conformally invariant. Setting s equal to zero in (45) and using equation (39) we find the required statement,

$$\frac{\delta c_{d/2}[\lambda^2 g]}{\delta \lambda(x)} = 0, \tag{46}$$

a result incidental to our present purpose, but useful later.

In a static space-time we can, as before, remove the time integration in tr_4 and get the reduced formula

$$\frac{\delta \operatorname{tr}_{3} \boldsymbol{\zeta}(s, \lambda^{2} g)}{\delta \lambda(\boldsymbol{x})} = 2s\lambda(\boldsymbol{x})g^{1/2}(\boldsymbol{x})(\boldsymbol{x}, t | \boldsymbol{\zeta}(s, \lambda^{2} g) | \boldsymbol{x}, t)$$
(47)

where the conformal factor is assumed to be a function of only the spatial coordinates.

The idea now is to use (47) to expand $tr_3 \zeta(s, \lambda^2 g)$ about the point $\lambda = 1$. To first order in $\ln \lambda$ we have

$$\operatorname{tr}_{3}\zeta(s,\lambda^{2}g) = \operatorname{tr}_{3}\zeta(s,g) + \int dx \frac{\delta \operatorname{tr}_{3}\zeta(s,\lambda^{2}g)}{\delta \ln \lambda(x)}\Big|_{\lambda=1} \ln \lambda(x)$$
(48)

so that from (47)

$$\operatorname{tr}_{3}\boldsymbol{\zeta}(s,\lambda^{2}g) - \operatorname{tr}_{3}\boldsymbol{\zeta}(s,g) = 2s \int \mathrm{d}\boldsymbol{x} \, g^{1/2}(\boldsymbol{x},t) |\boldsymbol{\zeta}(s,g)|\boldsymbol{x},t) \ln \lambda(\boldsymbol{x}) + D_{s}, \tag{49}$$

where D_s is the remainder. If λ is constant it is easily checked that D_s is zero so that D_s must depend only on the gradient of λ ,

$$D_s = D_s[\nabla\lambda, g]$$
 with $D_s[0, g] = 0$

and

$$D_0[\nabla\lambda, g] = 0.$$

We now interpret $g_{\mu\nu}$ as the optical metric $\bar{g}_{\mu\nu}$ and choose $\lambda^2 = g_{00}$ so that $\lambda^2 g_{\mu\nu}$ in (49) is the original general, static metric. Reverting to our previous notation, setting

 $s \rightarrow s - 1$ in (49) and dividing by (s - 1) we find, if (14) is referred to,

$$\bar{L}_{\infty}^{(1)} - L_{\infty}^{(1)} = -\frac{1}{2} \mathrm{i} \int \mathrm{d}\boldsymbol{x} \, \bar{g}^{1/2}(\overline{\boldsymbol{x}, t} | \boldsymbol{\tilde{\zeta}}(0, \infty) | \overline{\boldsymbol{x}, t}) \ln g_{00} + D_0'[\boldsymbol{\nabla} g_{00}, \boldsymbol{\tilde{g}}]$$
(50)

where \bar{D}_0' is the contribution from the D_s remainder.

All the ingredients are now to hand to construct the renormalised free energy, F_{ren} . Firstly we decide on the subtraction needed to turn F into F_{ren} . The divergence in F is the divergence in $F(\infty)$ which is the divergence in $-L_{\infty}^{(1)}$. From (33) this last is a pole at s = 1 with residue proportional to tr₃ $\zeta(0, \infty)$. If the conformal invariance of the zeta function at s = 0 is used (see equations (46), (47)) this residue is also proportional to the corresponding quantity in the optical metric, $\overline{\text{tr}_3} \overline{\zeta}(0, \infty)$, so that the divergence in $L_{\infty}^{(1)}$ is the same as that in $\overline{L}_{\infty}^{(1)}$. Therefore F diverges in the same way that \overline{F} does and we can write, from (43), (44)

$$F_{\rm ren} = \bar{L}_{\infty}^{(1)} - L_{\infty}^{(1)} + \bar{F}_{\rm ren}$$
(51)

so, if (41) and (50) are combined,

$$F_{\rm ren} = -\frac{\pi^2}{90} \frac{\bar{c}_0}{\beta_0^4} - \frac{\zeta_{\rm R}(3)}{4\pi^{3/2}} \frac{\bar{c}_{1/2}}{\beta_0^3} - \frac{1}{24} \frac{\bar{c}_1}{\beta_0^2} - \bar{\rm tr}_3 \,\bar{\boldsymbol{\zeta}}'_3(0,\infty) \frac{1}{2\beta_0} + \frac{\bar{c}_{3/2}}{8\pi^{3/2}} \frac{1}{\beta_0} \ln\beta_0 - \frac{\gamma}{16\pi^2} \bar{c}_2 + i \int d\boldsymbol{x} \,\bar{\boldsymbol{g}}^{1/2} (\bar{\boldsymbol{x}}, t) \bar{\boldsymbol{\zeta}}(0,\infty) |\bar{\boldsymbol{x}}, t\rangle \ln\left(\frac{\beta}{4\pi}\right) + \bar{D}'_0 - \frac{\pi^{3/2}}{16} \sum_{l=5/2}^{\infty} \bar{c}_l \Gamma(l - \frac{3}{2}) \boldsymbol{\zeta}_{\rm R}(2l - 3) \pi^{-2l} \left(\frac{\beta_0^2}{4}\right)^{l-2},$$
(52)

an expression valid for large temperatures. The main effect of going from \overline{F} to F has been to change the constant, β_0 , in the \overline{c}_2 term into $\beta = \beta_0 g_{00}^{1/2}$, the Tolman (inverse) temperature.

If we had chosen $g_{\mu\nu}$ in (49) as the original static metric and $\lambda^2 g_{\mu\nu}$, with $\lambda^2 = g_{00}^{-1}$, as the optical metric, which we could have done, equation (50) would have read

$$\bar{L}_{\infty}^{(1)} - L_{\infty}^{(1)} = -\frac{1}{2} \mathbf{i} \int d\mathbf{x} \, g^{1/2}(\mathbf{x}, t) |\boldsymbol{\zeta}(0, \infty)| \mathbf{x}, t) \ln g_{00} + D_0'(\nabla g_{00}^{-1}, g)$$

In this case the relevant terms in (52) would be

$$i \int d\boldsymbol{x} g^{1/2}(\boldsymbol{x}, t | \boldsymbol{\zeta}(0, \infty) | \boldsymbol{x}, t) \ln (\boldsymbol{\beta}/4\pi) + D'_0.$$
(53)

The high-temperature expansions for E_{ren} and S_{ren} can be quickly obtained from (42*a*), (42*b*) in similar fashion to F_{ren} , or direct from (52). We do not write them down since the only change from (42*a*) is that β_0 has become β in the \bar{c}_s term and there is an extra \bar{D}'_0 . Curiously the entropy depends only on the optical metric ($S(\infty) = 0$).

In order to determine the precise nature of the remainder term D_s it is necessary to examine the conformal transformation more closely. The analysis becomes quite complicated and there does not seem to be any closed formula. In this paper we shall leave the expressions as they are and return to a more exact treatment at another time. If g_{00} is only a slowly varying function of x then D'_0 will be small.

Regarding the form of the expansion (52) we recognise the first term as the usual Planck distribution with $\bar{c}_0 = \int d\mathbf{x} \, \bar{g}^{1/2} = |\bar{\mathcal{M}}_3|$, the Riemannian volume of $\bar{\mathcal{M}}_3$ or, equivalently, the optical volume of \mathcal{M}_3 .

If we formally define a free energy density f(x) by

$$F = \int \mathrm{d}\boldsymbol{x} \, g^{1/2} \, f(\boldsymbol{x})$$

then the first term of (52) gives a contribution to $f(\mathbf{x})$ of the form

$$f_{\rm Planck} = -\frac{\pi^2}{90}\beta^{-4}$$

which depends solely on the local Tolman temperature. The other terms in (52) involving only powers of β_0 can likewise be expressed in terms of β . This follows by explicit construction of the \bar{c} coefficients, or from just their scaling properties or from the general scaling property of F,

$$F_{\beta_0}[\alpha^2 g_{00}] = \alpha F_{\alpha\beta_0}[g_{00}], \qquad \alpha = \text{constant}$$

This scaling rule must be true but it is instructive to check it term by term in (52). It is valid for the $\ln(\beta/4\pi)$ plus the D' terms by virtue of (49) and (22). The term needed to provide the scaling of the $\bar{c}_{3/2} \ln \beta_0$ term comes from $\overline{\text{tr}}_3 \bar{\zeta}'_3(0, \infty)$. We leave the details as an exercise to the reader.

If one wishes, one can think of the terms in (52), apart from the first one, as being corrections to the Planck form due to curvature and boundary effects. To specify them more closely the precise expressions for the coefficients \bar{c}_l are required. As has been mentioned, if $\bar{\mathcal{M}}_3$ has no boundary, $\partial \bar{\mathcal{M}}_3 = \emptyset$, all the $\bar{c}_{(2l+1)/2}$ vanish, and explicit forms for the volume parts $\bar{a}_1(x, x)$, $\bar{a}_2(x, x)$ and $\bar{a}_3(x, x)$ (refer to equation (36)) have been found, the first two by DeWitt (1965) (see also Christensen 1976) and the third by Sakai (1971), in terms of the local curvature of $\bar{\mathcal{M}}_3$. More general expressions and formulae can be found in the work of Gilkey (1975a, b).

In our case $\bar{a}_1(x, x)$ will vanish due to the choice of a conformally invariant equation, (1), while the expression for $a_2(x, x)$ can be found, by now, in many places since it is the coefficient which enters into the conformal trace anomaly (Dowker and Critchley 1977b).

If \mathcal{M}_3 is flat (this means that \mathcal{M} is conformally flat) the most general explicit results for the \tilde{c}_i seem to be those of Waechter (1972) and the more formal ones of Greiner (1971) and Seeley (1967). (See also Gilkey (1975c).) Some of these results are summarised by Baltes and Hilf (1976) where further references can be found, particularly to the derivation of the so called 'edge' and 'corner' terms which are needed for non-smooth boundaries.

Writing the \bar{c}_l as in equation (36), the explicit forms for the first few boundary parts \bar{b}_l are (e.g. Brownell 1957, McKean and Singer 1967, Waechter 1972), for a smooth, convex boundary

$$\bar{b}_{1/2} = -\frac{1}{2}\pi^{1/2} |\partial \bar{\mathcal{M}}_3| \tag{54a}$$

$$\bar{b}_1 = \frac{1}{3} \int d\bar{\sigma} (\bar{\kappa}_1 + \bar{\kappa}_2)$$
(54b)

$$\bar{b}_{3/2} = \frac{\pi^{1/2}}{64} \int d\bar{\sigma} (\bar{\kappa}_1 - \bar{\kappa}_2)^2$$
(54c)

where $\bar{\kappa}_1$ and $\bar{\kappa}_2$ are principle curvatures of $\partial \bar{\mathcal{M}}_3$, and $|\partial \bar{\mathcal{M}}_3|$ is the Riemannian volume

(surface area) of $\partial \tilde{\mathcal{M}}_3$, and equals $\int d\bar{\sigma}$. The coefficient \bar{b}_1 may be expressed alternatively as

$$\vec{b}_1 = \frac{1}{3} \int \mathrm{d}\vec{\sigma} \, \vec{g}^{ij} \, \vec{\Omega}_{ij}$$

i.e. one third of the integrated trace of the second fundamental form, $\overline{\Omega}$, of $\partial \overline{\mathcal{M}}_3$ (see, e.g., Eisenhart 1926, p 158, problem 2), a form valid for any dimension. We should perhaps note that (54c) has been proved for a flat $\overline{\mathcal{M}}_3$ only.

For the sphere in flat three-space Waechter (1972) has given all the \bar{c}_l up to $\bar{c}_{5/2}$; $\bar{c}_{3/2}$ vanishes as is seen from (54c) but \bar{c}_2 does not.

Case and Chiu (1970) have performed the electromagnetic energy mode sum in a cube and obtained an expansion similar to (42a), but without a $\ln \beta_0$ term. The first few terms agree numerically with (42a), allowing for the different physical systems. A similar statement is true also for the sphere (Baltes and Hilf 1976).

Apart from these high-temperature expansions we can use a general sum-overstates form like (31). Thus

$$F = F(\infty) + \bar{F}' = F(\infty) + \beta_0^{-1} \sum_{\omega_k} d_k \ln(1 - e^{-\beta_0 \omega_k})$$
(55)

with, from (25), $F(\infty)$ given by the negative of the expression in equation (33), for $\beta_0 = \infty$. Taking the same renormalisation prescription as before yields

$$F_{\rm ren} = \beta_0^{-1} \sum_{\omega_k} d_k \ln(1 - e^{-\beta_0 \omega_k}) + \frac{1}{2} i \, {\rm tr}_3 \, \boldsymbol{\zeta}'(0, \infty)$$
(56)

as the appropriate low-temperature form. This then yields the energy and entropy:

$$E_{\rm ren} = \sum_{\omega_k} \omega_k (e^{\beta_0 \omega_k} - 1)^{-1} d_k + E_{\rm ren}(\infty)$$
(57*a*)

$$S_{\rm ren} = \sum_{\omega_k} d_k [\beta_0 \omega_k (e^{\beta_0 \omega_k} - 1)^{-1} - \ln(1 - e^{-\beta_0 \omega_k})]$$
(57b)

with, of course,

$$E_{\rm ren}(\infty) = F_{\rm ren}(\infty)$$

A low-temperature expansion for F analogous to (52) for high temperatures can be given in terms of the function that describes the distribution of eigenvalues, $N(\omega)$, (the mode function, e.g., Brownell 1957, Clark 1967, Baltes and Hilf 1976, Balian and Bloch 1970, 1971), for small ω . $N(\omega)$ is defined by

$$N(\omega) = \sum_{\omega_k < \omega} d_k + \sum_{\omega_k = \omega} \frac{1}{2} d_k$$

such that the density of eigenvalues $\rho(\omega)$,

$$\rho(\omega) = \sum_{k} \delta(\omega - \omega_{k}),$$

is equal to $dN/d\omega$. Then we can write

$$F = \beta_0^{-1} \int_0^\infty \ln(1 - e^{-\beta_0 \omega}) \frac{\mathrm{d}N}{\mathrm{d}\omega} \mathrm{d}\omega + F(\infty).$$
(58)

Large β_0 means that small ω is the most important region and, writing a Taylor series

for $dN/d\omega$,

$$dN(\omega)/d\omega = \sum_{n=0}^{\infty} \omega^n (n!)^{-1} N^{(n+1)}(0) + \text{remainder},$$

we find

$$F = F(\infty) - \sum_{n=0}^{\infty} \beta_0^{-n-2} N^{(n+1)}(0) \zeta_{\rm R}(n+2) + \text{remainder}.$$
 (59)

Strictly speaking, for entirely discrete modes, $dN/d\omega$ will be all 'remainder' i.e. all the $N^{(n)}(0)$ will be zero and there will be no powers of T in the low-T expansion. However, if the system is non-compact, so that there is a continuous eigenvalue running down to $\omega = 0$, some of the $N^{(n)}(0)$ will be non-zero. For example, in the parallel-plate Casimir geometry $N^{(1)}(\omega)$ has a contribution

$$\int \int \mathrm{d}k_1 \, \mathrm{d}k_2 \, \delta(\omega - (k_1^2 + k_2^2)^{1/2}) \sim \omega$$

so that $N^{(2)}(0)$ is non-zero giving a correction to F (and E) which goes like T^3 , as found by Mehra (1967) and Brown and Maclay (1969). The reader can check that the cylinder gives a T^2 behaviour.

5. Renormalisation and boundary effects

We turn now to the question of renormalisation, that is, to the extraction of physically significant finite answers. What one does depends on the questions one asks. For example, it seems to be necessary to specify what is the significance of the boundary, ∂M_3 . Two basic situations can be envisaged: (a) ∂M_3 is actually the limit of physical reality so that there is no outside, no 'other side', of ∂M_3 ; and (b) ∂M_3 divides a larger manifold M'_3 into two parts, M_3 and its closure M^*_3 , so that

$$\mathcal{M}_3' = \mathcal{M}_3 \cup \mathcal{M}_3^*.$$

(Strictly speaking we should include ∂M_3 in M'_3 since M_3 and M''_3 are taken as open sets. We assume that ∂M_3 has no thickness.)

Clearly the nature of the boundary will be reflected in the boundary conditions on the fields. In the present paper we did not wish to become involved with questions of physically realistic boundary conditions and simply chose D or N conditions on ϕ , which implies that there is no flux, of $\overline{\phi}$, or ϕ , across $\partial \overline{M}_3$, or ∂M_3 .

Up to now we have been implicitly concentrating on case (a) where (43) would give the 'intrinsic', unrenormalised free energy F of the system contained in \mathcal{M}_3 and (33) the effective Lagrangian $L_{\beta_0}^{(1)}$. The renormalisation we used for $L_{\beta_0}^{(1)}$, and therefore for F, was to drop the pole term in (33). This procedure is equivalent to defining Det G_{β_0} to be $\exp(tr_4 \zeta'(0, \beta_0))$ which is certainly very reasonable (Hawking 1977, Gibbons 1977) and gives the right answers, when these are known. Such a definition avoids any questions of renormalisation because the infinities have been defined away.

However convenient or economical this may be, it is probably better to keep the pole terms and argue them away by an explicit renormalisation, if possible, although the final result will probably be the same.

Conventionally (e.g. DeWitt 1965, 1975, Utiyama and DeWitt 1962) the a_2 part of the c_2 pole (remember that $\operatorname{tr}_3 \zeta(0, \infty) = i(16\pi^2)^{-1}c_2$ where the c_l are the

coefficients in the expansion of tr₃ $K_{\infty}(\tau)$) in (33) is absorbed by a renormalisation of a quadratic term introduced into the free gravitational action for just this purpose. Similarly, for consistency, the removal of the boundary part b_2 (see equation (36) and recall that $\bar{c}_2 = c_2$), ought to correspond to the renormalisation of some surface gravitational action. Dimensional arguments show that the analogue of the quadratic volume action, $\int R^2 g^{1/2} d^4 x$, is typically a $\int \operatorname{tr} \Omega^3 dt d\sigma$ term (tr here just means matrix trace). Gibbons and Hawking (1977) have recently emphasised the role of surface terms in the gravitational action, the usual $\int_{\mathcal{M}} R g^{1/2} d^4 x$ part being augmented by a $\int_{\mathcal{M}} \operatorname{tr} \Omega d\Sigma$ term.

Our final comment on case (a) is that there is still, of course, the possibility of further finite renormalisations.

Turning now to case (b) the first question which springs to mind is the one Casimir asked. Given a large enclosure \mathcal{M}'_3 at temperature β_0^{-1} , what is the global effect of introducing a boundary $\partial \mathcal{M}_3$? This is easily expressed as the difference in free energy before and after constructing the boundary:

$$\Delta F = F(\mathcal{M}_3) + F(\mathcal{M}_3^*) - F(\mathcal{M}_3'). \tag{60}$$

A similar technique was used by Lukosz (1973a, b) in the zero-temperature case for the internal energy.

F in (60) is the unrenormalised free energy and (60) is a statement of 'Casimir renormalisation'. We note that ΔF is not intrinsic to either \mathcal{M}_3 or \mathcal{M}_3^* but is an attribute of the entire manifold.

Let us consider the high-temperature expansion of ΔF . For each term in (60) there will be an expansion like (52), or (41) for the ultrastatic case which we consider from now on for simplicity.

Firstly note that the outer boundary of \mathcal{M}_3^* is the boundary of \mathcal{M}_3' , $\partial \mathcal{M}_3'$. Thus the contributions from $\partial \mathcal{M}_3'$ in the last two terms of (60) cancel. Further, all the volume terms, a_l , in the three expansions cancel since

$$a_{l}(\mathcal{M}_{3})+a_{l}(\mathcal{M}_{3}^{*})=a_{l}(\mathcal{M}_{3}\cup\mathcal{M}_{3}^{*}).$$

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In addition, the surface contributions, b_l , have the property, for smooth boundaries,

$$b_l(-\partial \mathcal{M}_3) = (-1)^{2l+1} b_l(\partial \mathcal{M}_3) \tag{61}$$

and, on noting that the inner boundary of \mathcal{M}_3^* is the boundary of \mathcal{M}_3 but oppositely oriented, $-\partial \mathcal{M}_3$, the high-temperature expansion for the Casimir free energy $\Delta \vec{F}$ is

$$\Delta \bar{F} = -\frac{\bar{b}_{1/2}}{2\pi^{3/2}} \frac{\zeta_{\mathbf{R}}(3)}{\beta_0^3} + \frac{\bar{b}_{3/2}}{4\pi^{3/2}} \frac{1}{\beta_0} \ln \beta_0 - \frac{\pi^{-3/2}}{8} \sum_{n=1}^{\infty} \bar{b}_{(2n+3)/2} \frac{(n-1)!}{(2n)!} \beta_0^{2n-1} |B_{2n}| -\frac{1}{2\beta_0} (\bar{\zeta}'_3(0,\mathcal{M}_3) + \bar{\zeta}'_3(0,\mathcal{M}_3^*) - \bar{\zeta}'_3(0,\mathcal{M}'_3))$$
(62)

where the $\bar{b_l}$ are evaluated for the boundary $\partial \bar{\mathcal{M}}_3$, and we have simplified the notation by dropping the tr₃ and the β dependence of the $\bar{\zeta}'_3$ terms.

We see that the Casimir renormalisation has eliminated the \bar{c}_2 pole.

If the boundary were flexible it would adjust its shape and size so as to minimise $\Delta \overline{F}$. For a dominant first term in (62) the Casimir stresses would try to increase the boundary surface area (see equation (54*a*)). If the second term were at all appreciable, or if the electromagnetic case were being considered, for which the $\overline{b}_{1/2}$ term does not arise, the stresses would tend to distort the shape of ∂M_{3} .

To see this note that the expression (54c) for $\vec{b}_{3/2}$ (in flat space for scalar fields) is unchanged under re-scaling of distances on $\partial \bar{\mathcal{M}}_3$ and so is purely shape dependent. Use of the standard results

$$\int_{\partial \bar{\mathcal{A}}_3} \mathrm{d}\bar{\sigma} \,\bar{\kappa}_1 \bar{\kappa}_2 = 4\pi\chi = 4\pi(p-h)$$

where χ is the Euler characteristic of the surface, p its number of disconnected parts, i.e.

$$\partial \mathcal{M}_3 = \bigcup_{i=1}^p \partial \mathcal{M}_{3i}$$

and h its total number of holes, yields the expression

$$-\frac{1}{32} \left(\frac{1}{8\pi} \int d\tilde{\sigma} \operatorname{tr} \bar{\Omega}^2 + (h-p) \right) \beta_0^{-1} \ln \beta_0^{-1}$$

for the $\overline{b}_{3/2}$ term in ΔF . The surface will try to adjust itself so that the first term in the bracket is a maximum, assuming that the deformation does not alter the topology. For example, $\overline{b}_{3/2}$ is zero for a sphere but becomes positive if the sphere develops a 'spare tyre' bulge around the equator.

If the boundary has sharp edges and corners (61) no longer holds and the cancellations are not complete. In particular there is probably a residual boundary pole $\Delta \bar{b}_2/(s-1)$. We say probably because the expressions for b_2 have not been evaluated yet.

A similar general conclusion is reached by Lukosz (1973a, b) who uses a different method of regularisation and works at zero temperature. Essentially he uses point splitting, in the guise of a high-frequency cut-off. This yields a residual divergence in the Casimir energy which, dimensionally, goes like $\Delta \bar{b}_1 / \delta^2$ where δ is the small distance introduced by the cut-off. Presumably if Lukosz's calculation were taken further it would produce a residual divergence $\Delta \bar{b}_2 \ln \delta$, to compare with the zeta function form $\Delta \bar{b}_2 / (s-1)$.

(This difference in number, and form, of divergences, is typical of the two regularisation methods. It is well known that point splitting produces, in the absence of boundaries, three sorts of divergence, of the order of $c_0\delta^{-4}$, $c_1\delta^{-2}$ and $c_2 \ln \delta$, while the zeta function and dimensional regularisations give only a $c_2/(s-1)$ pole. Usually this difference is of no account since the infinities are renormalised away leaving identical finite parts.)

Lukosz (1973a, b) does not resolve the problem of the residual divergence except to say, quite reasonably, that sharp edges and corners are unphysical anyway.

Apart from this question mark, the Casimir renormalisation seems quite reasonable and suitable for the situation it seeks to cover. There is, however, another point of view. Instead of taking the F's in (60) to be unrenormalised, one takes them to be the renormalised ones, and defines

$$\Delta F_{\rm ren} = F_{\rm ren}(\mathcal{M}_3) + F_{\rm ren}(\mathcal{M}_3^*) - F_{\rm ren}(\mathcal{M}_3'). \tag{63}$$

This combination is then no longer a means of rendering anything finite. It is simply a result of applying the case (a) attitude to each region. ΔF_{ren} will be finite even if there are edges and corners. It equals ΔF for smooth boundaries.

Further light might be thrown on the divergence problem by looking at local quantities and this forms the subject of the next subsection.

5.1. Local questions

So far we have been concerned mainly with integrated quantities such as the total free energy and the Lagrangian. Consider now the problem of determining the local averaged stress-energy tensor density. If the Lagrangian is known as a functional of the general static metric then a functional differentiation, equation (1), yields the answer. Alternatively the explicit form of $T_{\mu\nu}$ can be used. As an example we choose T_{00} and it is then easy to show, using Parker's (1973) conformal relation for the conformal stress tensor, that $\langle \hat{T}_{00} \rangle$ is given as the coincidence limit,

$$\langle \hat{T}_{00}(\boldsymbol{x}) \rangle = \mathrm{i} g^{00}(\boldsymbol{x}) \lim_{\boldsymbol{x}' \to \boldsymbol{x}} \left[\partial_0 \partial_0 + \frac{1}{6} (\bar{\nabla}^i \bar{\nabla}_{i'} + \bar{\nabla}^i \bar{\nabla}_i) \right] \bar{G}_{\beta_0}(\boldsymbol{x}, \boldsymbol{x}'), \tag{64}$$

where the bars refer to the optical metric and \bar{G}_{β_0} is given by $g_{00}^{1/2}G_{\beta_0}g_{00}^{\prime 1/2}$.

This particular form is not really needed for the points we wish to make just now, but is given for reference. All we need to know is that $\langle \hat{T}_{00} \rangle$ is given as the coincidence limit of some differential operator acting on the finite-temperature Green function. This can be expressed briefly as

$$\langle \hat{T}_{00} \rangle = [\hat{T}_{00} G_{\beta_0}].$$
 (65)

 $\langle \hat{T}_{00} \rangle$ diverges and so some prescription, which we shall term 'renormalisation', for making it finite is needed. One possibility, used by a number of people, including Brown and Maclay (1969), Candelas and Raine (1976), Candelas and Deutsch (1977) and Dowker and Critchley (1976b), in the case that the space-time is flat, is to write

$$G_{\beta_0}(\mathcal{M}) = G_{\beta_0}(\mathcal{M}') + G'_{\beta_0}(\mathcal{M}) \tag{66}$$

where $G_{\beta_0}(\mathcal{M}')$ is the Green function for the complete space-time \mathcal{M}' , without the boundary, $\partial \mathcal{M}_3$. In other words it is the 'Minkowski finite-temperature Green function' given as the image sum,

$$G_{\beta_0}(x, x', \mathcal{M}') = \sum_{m=-\infty}^{\infty} G_{\infty}(x, x' - i\lambda m\beta_0, \mathcal{M}'), \qquad (67)$$

where $G_{\infty}(x, x')$ is the usual Green function $(= -i/4\pi^2 \sigma^2)$, but we do not need the exact form). The $G'_{\beta_0}(\mathcal{M}; \partial \mathcal{M}_3)$ is the correction term due to boundary effects.

The renormalisation adopted by the above authors is to drop the Minkowski (zero-temperature) Green function in (67), i.e. the m = 0 term. This gives a subtracted 'Green function':

$$G_{\beta_0}^{\text{sub}}(x, x', \mathcal{M}') = \sum_{m=-\infty}^{\infty'} G_{\infty}(x, x' - i\lambda m\beta_0, \mathcal{M}')$$
(68)

which is put into (66) to give a $G_{\beta_0}^{\text{sub}}(\mathcal{M})$ which, in turn, is used in (65) to produce a finite $\langle \hat{T}_{00} \rangle_{\text{ren}}^{\mathcal{M}}$,

$$\langle \hat{T}_{00} \rangle_{\text{ren}}^{\mathcal{M}} = [\vec{T}_{00}(G_{\beta_0}^{\text{sub}}(\mathcal{M}') + G_{\beta_0}'(\mathcal{M}, \partial \mathcal{M}_3))].$$
(69)

This quantity is supposed to have physical significance.

If the space-time is curved then the renormalisation is more complicated than simply dropping the m = 0 term in (67). One would have to have recourse to point splitting, dimensional regularisation or a local zeta function method. At the moment this would only complicate matters.

An analogous equation to (69) holds with \mathcal{M}_3 replaced by its closure \mathcal{M}_3^* . For simplicity we write this as $\mathcal{M} \rightarrow \mathcal{M}^*$.

To try to make contact with the global quantities considered earlier these densities can be integrated. Firstly we construct the Casimir energy ΔE (cf (60)) from the unrenormalised densities (65):.

$$\Delta E = \int_{\mathcal{M}_{3}} d\mathbf{x} [\vec{T}_{00}(G_{\beta_{0}}(\mathcal{M}') + G'_{\beta_{0}}(\mathcal{M}, \partial\mathcal{M}_{3}))] + \int_{\mathcal{M}_{3}} d\mathbf{x} [\vec{T}_{00}(G_{\beta_{0}}(\mathcal{M}') + G'_{\beta_{0}}(\mathcal{M}^{*}, -\partial\mathcal{M}_{3}))] - \int_{\mathcal{M}_{3}} d\mathbf{x} [\vec{T}_{00}G_{\beta_{0}}(\mathcal{M}')]$$
(70)
$$= \int_{\mathcal{M}_{3}} d\mathbf{x} [\vec{T}_{00}G'_{\beta_{0}}(\mathcal{M}, \partial\mathcal{M}_{3})] + \int_{\mathcal{M}_{3}} d\mathbf{x} [\vec{T}_{00}G'_{\beta_{0}}(\mathcal{M}^{*}, -\partial\mathcal{M}_{3})].$$
(71)

It is easily seen that this result is unchanged if the renormalised densities of (69) are used since the renormalisation affects only the complete manifold, \mathcal{M}' , quantities, and these cancel. The difference is that in the global Casimir renormalisation no significance is attached to the local densities.

Asymptotic expressions for $\langle \hat{T}_{00} \rangle$ have been derived by Deutsch and Candelas (private communication) and later by Critchley. They show a divergence with a leading term of the order of d^{-3} as the boundary is approached, where d is the distance from the boundary. The coefficient is proportional to $(\kappa_1 + \kappa_2)$ so that the density reverses sign on the other side of the boundary. If this leading term is integrated over a thin shell surrounding the boundary there is a cancellation of the strongest divergence but infinities of the form δ^{-1} and $\ln \delta$, as $\delta \to 0$, still remain (δ has dimensions of length). To see whether these can be removed also, one needs more terms in the expansion of $\langle \hat{T}_{00} \rangle$ in powers of d^{-1} . Deutsch (private communication) has evaluated the term of order d^{-2} . Unfortunately the next term at least is needed as well.

Even if there should be a cancellation between the inside and outside, the intrinsic renormalised energy will diverge due to the d^{-3} behaviour near the boundary. By contrast the total intrinsic energy evaluated by the zeta function method earlier is finite, after eliminating the c_2 pole.

As we see it there are several ways of viewing this situation.

(i) The total energy really is infinite. This is because of the unphysical nature of the assumed boundary conditions, a point of view adopted by Deutsch and Candelas.

(ii) The local method gives the correct density at any strictly internal point but breaks down on ∂M_3 . There is then a 'surface contribution' which makes the total energy finite. The energy density still tends to infinity as the boundary is approached and it is this particular local effect that is to be thought of as caused by the unphysical boundary conditions.

It might be thought that since the subtraction procedure in the local approach subtracted off only the Minkowski expression one should, in fairness, remove only the a_2 part of the c_2 pole in the zeta function method (actually a_2 is zero for flat space-time anyway). This would leave the boundary part $b_2/(s-1)$ (which is in general non-zero), as a divergence.

Such a possibility can be ruled out by considering the case of the cubic cavity for which, although it does not have a smooth boundary, $\langle \hat{T}_{00} \rangle$ still diverges as the corners are approached so as to render the integrated $\langle \hat{T}_{00} \rangle$ infinite (Dowker, unpublished). However in this case c_2 is zero. In fact, rectangular cavities provide more or less explicitly soluble examples of some of these ideas and in the next section we consider

in more detail the infinite waveguide of rectangular (actually square) cross section in Minkowski space-time, with Dirichlet boundary conditions.

6. The infinite waveguide

We concentrate on the zero-temperature case for which the total internal energy E is equal to the negative of the effective Lagrangian, according to (25), so that in terms of the spatially integrated space-time zeta function, tr₃ $\zeta_4(s)$ (see equation (15)),

$$E = \frac{i}{2} \lim_{s \to 1} \frac{[tr_3 \zeta_4(s)]}{s-1} = \frac{i}{2} \left(\frac{[tr_3 \zeta_4(0)]}{s-1} + [tr_3 \zeta_4'(0)] \right)$$

where the square brackets have been inserted to emphasise that a time coincidence limit has been taken.

For ultrastatic space-times, $[\zeta_4(s)]$ can be related to the zeta function on the spatial section, the $\zeta_3(s)$ introduced in § 3. The relation is easily found to be

$$[\boldsymbol{\zeta}_4(s)] = \frac{i}{(4\pi)^{1/2}} \frac{\Gamma(s-\frac{1}{2})}{\Gamma(s)} \boldsymbol{\zeta}_3(s-\frac{1}{2}).$$
(72)

In general tr₃ $\zeta_3(s)$ has poles at $s = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, \ldots$

For the infinite waveguide of constant cross-sectional size and shape it is necessary to deal with a unit length along the guide and to remove the corresponding integration. Then $[\zeta_3(s)]$ can be related to $\zeta_2(s)$, where $\zeta_2(s)$ is the zeta function for the cross section domain of the guide and the square brackets now stand for a coincidence limit on the z coordinate, if the guide is along the z axis. We have

$$[\boldsymbol{\zeta}_3(s)] = (4\pi)^{-1/2} \frac{\Gamma(s-\frac{1}{2})}{\Gamma(s)} \boldsymbol{\zeta}_2(s-\frac{1}{2})$$

and, combining the above results, the energy per unit length of the guide is given by

$$E = +\frac{1}{8\pi} \left(\frac{\operatorname{tr}_2 \, \boldsymbol{\zeta}_2(-1)}{s-1} + \operatorname{tr}_2 \, \boldsymbol{\zeta}_2(-1) + \operatorname{tr}_2 \, \boldsymbol{\zeta}_2'(-1) \right). \tag{73}$$

The particular values $\operatorname{tr}_d \zeta_d(-n)$ are related to the expansion coefficients $c_{(\frac{1}{2}d+n)}$ (see Minakshisundaram and Pleijel 1949). Here, $\operatorname{tr}_2 \zeta_2(-1)$ is proportional to c_2 , and this is zero for the rectangle (e.g. Waechter 1972, Brownell 1957). We shall verify this shortly.

For Dirichlet boundary conditions the integrated zeta function for the rectangle of sides a and b is

$$\operatorname{tr}_{2} \zeta_{2}(s) = \pi^{-2s} \sum_{l,m=1}^{\infty} \left[\left(\frac{l}{a} \right)^{2} + \left(\frac{m}{b} \right)^{2} \right]^{-s}.$$

Unfortunately for general a and b this cannot be given in closed form but special cases are known. For the square, a = b, Hardy (1919) has given

$$\sum_{l,m=-\infty}^{\infty} {{'}}{{(l^{2}+m^{2})}^{-s}} = 4\zeta_{\rm R}(s)\beta(s)$$

where

$$\beta(s) = \sum_{n=0}^{\infty} (-1)^n (2n+1)^{-s}, \qquad s > 2$$

which can be continued to the whole s plane to yield the β function. Thus,

$$\operatorname{tr}_{2}\zeta_{2}(s) = (a/\pi)^{2s}(\zeta_{\mathsf{R}}(s)\beta(s) - \zeta_{\mathsf{R}}(2s))$$

where the last term in brackets allows for the non-appearance of terms with either l or m zero.

If s is set equal to -1 and the values $\zeta_{\mathbf{R}}(-2) = 0 = \beta(-1)$ are recalled we have

 $\operatorname{tr}_2 \boldsymbol{\zeta}_2(-1) = 0$

as promised. There is no pole in the rectangular case. This is not true for the circle, for example, because c_2 is not zero (Waechter 1972).

The β function satisfies the functional relation (Hardy 1949)

$$\beta(s) = \Gamma(1-s)(\pi/2)^{s-1} \cos(\pi s/2)\beta(1-s)$$

from which we can deduce that

$$\beta'(-1) = (2/\pi)\beta(2)$$

where $\beta(2) = 0.915965...$ is Catalan's constant. Similarly we find for the Riemann zeta function

$$\zeta'_{\mathsf{R}}(-2) = -(2\pi)^{-2} \zeta_{\mathsf{R}}(3), \qquad \zeta_{\mathsf{R}}(-1) = -(2\pi^{2})^{-1} \zeta_{\mathsf{R}}(2).$$

If these values are substituted into (73) there results

$$E_{\rm ren} = E = -(8\pi^2 a^2)^{-1} (\zeta_{\rm R}(2)\beta(2) - \frac{1}{2}\pi\zeta_{\rm R}(3)).$$
(74)

The numerical value of the term in brackets is -0.381 so that E is positive. For periodic boundary conditions there is no $\zeta_{\rm R}(3)$ term, and there is an overall factor of 2^4 . E is then negative.

Lukosz (1971, 1973a, b) has evaluated the Casimir effect for a cube, and rectangular waveguide by two methods—eigenvalue summation and images. The two methods agree except that in the image method there is still the problem of the residual edge divergences mentioned earlier. If these are ignored, Lukosz finds for the Casimir energy, E, just the first term in brackets of (74), which makes E negative. (We have to allow for an overall factor of 2 since Lukosz is considering electromagnetism).

The zeta function value for ΔE would be found by combining the renormalised energies as in (63). It can be argued that the outside (\mathcal{M}_3^*) effect is a purely divergent one. If this is so, and it is by no means obvious, we can identify the E of (74) with ΔE_{ren} since the energy of the total (\mathcal{M}'_3) tends to zero as the size tends to infinity. There would then be a discrepancy between Lukosz's result and ours, although there is still the possibility that the last term in (74) is cancelled by the effect of the exterior modes. We have not been able to show this. In his eigenvalue method, Lukosz (1971) explicitly says that the presence of the walls does not change the energy density outside.

It is interesting to note that exactly the $\zeta_{R}(3)$ term in (74) occurs in an image method (Dowker, unpublished) as being due to the effect of the images formed by an odd number of reflections. The zeta function method appears to give a specific

algorithm for dealing with the other images, a set of which are responsible for the divergence of $\langle \hat{T}_{\mu\nu} \rangle$ as the corners are approached.

Another rectangular cavity that can be explicitly dealt with is when b = 2a. One now has the sum

$$\sum_{l,m=1}^{\infty} (l^2 + 4m^2)^{-s} = \frac{1}{2}(1 - 2^{-s} + 2^{1-2s})\zeta_{\rm R}(s)\beta(s) - \frac{1}{2}(1 + 2^{-2s})\zeta_{\rm R}(2s)$$

and the calculation proceeds as above with the result

$$E = -(8\pi^2 A)^{-1} (\frac{7}{4} \zeta_{\rm R}(2)\beta(2) - \frac{5}{8}\pi \zeta_{\rm R}(3))$$
(75)

where $A = 2a^2$ is the cross-sectional area. The numerical value of the bracket is 0.2769 and so, on this theory anyway, as the cross section becomes more elongated the energy becomes more negative for the same area.

We can also roughly check that the change from (74) to (75) is in the right direction by comparing the average energy densities E/A. For the square we have

$$(E/A)_{b=a} = 0.381(8\pi^2 a^4)^{-1} \tag{76}$$

while

$$(E/A)_{b=2a} = -0.069(8\pi^2 a^4)^{-1}.$$

The average density is decreasing as the square waveguide elongates to the parallelplate geometry. This is correct because in the limit $b \rightarrow \infty$, the answer is the standard one (e.g. DeWitt 1975, Schwinger 1975)

$$(E/A)_{b=\infty} = -\pi^2 (1440a^4)^{-1} = -0.541(8\pi^2 a^4)^{-1}.$$

Unfortunately the explicit results (74), (75) cannot be extended to the local problem. In order to find the energy density $\langle \hat{T}_0^0 \rangle$ we require a closed form for the analytic continuation of the local zeta function in the rectangle:

$$(x, y|\boldsymbol{\zeta}_{2}(s)|x, y) = \sum_{l,m=1}^{\infty} \frac{\pi^{2-2s} \sin^{2}(lx\pi/a) \sin^{2}(my\pi/b)}{ab[(l^{2}/a^{2}) + (m^{2}/b^{2})]^{s}}, \qquad (x, y) \in \mathcal{M}_{2}.$$
(77)

 $\langle \hat{T}_0^0 \rangle$ is then given, up to a factor, by evaluating the derivative with respect to s at s = -1. (77), and its off-diagonal form, are Epstein zeta functions with known and relevant properties. Their uses for the rectangle and other cross-sectional manifolds, such as the Klein bottle and Möbius strip, are treated in a paper in preparation.

A result which it is sometimes useful to bear in mind, is that in an infinite wedge of angle α the renormalised stress tensor $\langle \hat{T}^{\mu\nu} \rangle_{ren}$ calculated on the basis of equation (69), for $\beta_0 = \infty$, is (Dowker 1976, unpublished)

$$\langle \hat{T}^{\mu\nu} \rangle_{\rm ren} = -\frac{1}{1440\alpha^2 r^4} \left(\frac{\pi^2}{\alpha^2} - \frac{\alpha^2}{\pi^2} \right) \begin{bmatrix} 1 & 0 & \\ & -1 & 0 & \\ & 0 & 3/r^2 & \\ & & & -1 \end{bmatrix},$$
 (78)

in cylindrical coordinates with 0 = t, 1 = r, $2 = \theta$ and 3 = z. Thus the energy density diverges negatively, if $\alpha < \pi$, as the edge of the wedge is approached, $r \rightarrow 0$. It is easily checked that (78) reduces to the parallel-plate value as α tends to zero and r to infinity in such a way that $\alpha r = a$ remains finite.

7. Scaling and trace anomalies

If the arbitrary scale length L or, equivalently, the renormalisation point or mass parameter (see e.g. Duff 1975, Brown 1977, Hawking 1977, Dowker and Critchley 1977b) is introduced the modification amounts to an additional $(16\pi^2)^{-1}c_2 \ln L$ term in, say, the $L_{\beta_0}^{(1)}$ of equation (15). This will turn the $\ln(\beta/4\pi)$ in the free energy (52) into $\ln(\beta/4\pi L)$, making the argument of the logarithm manifestly dimensionless. By contrast, the $c_{3/2} \ln \beta_0$ term acquires a scale from the ζ'_3 term. In any particular system if ζ'_3 could be evaluated one would find a term $-c_{3/2} \ln D$ where D is a typical dimension characterising the manifold ($\mathcal{M}_3, \partial \mathcal{M}_3$).

Changes of scale are related to conformal transformations and this seems to be the appropriate place to mention the conformal trace anomalies.

A standard formula gives the trace of the averaged stress tensor as

$$g^{\mu\nu}\langle \hat{T}_{\mu\nu}(\mathbf{x})\rangle = -g^{-1/2} \frac{\delta L^{(1)}_{\beta_0}[\lambda^2 g]}{\delta\lambda(\mathbf{x})}\Big|_{\lambda=1}$$
(79)

and for $L_{\beta_0}^{(1)}$ we use (14).

Since the conformal properties of G_{β_0} are the same as those of G_{∞} we derive the finite-temperature version of (47):

$$\frac{\delta \operatorname{tr}_{3} \boldsymbol{\zeta}(s, \lambda^{2} g, \beta_{0})}{\delta \lambda(\boldsymbol{x})} = 2s\lambda(\boldsymbol{x})g^{1/2}(\boldsymbol{x})(\boldsymbol{x}, t | \boldsymbol{\zeta}(s, \lambda^{2} g, \beta_{0}) | \boldsymbol{x}, t).$$

Whence with (79) and (14)

 $g^{\mu\nu}\langle \hat{T}_{\mu\nu}(\mathbf{x})\rangle = \mathbf{i}(\mathbf{x}, t|\boldsymbol{\zeta}(0, \beta_0)|\mathbf{x}, t).$ (80)

Now, for exactly the same reason that the pole in (15) can be replaced by the zero-temperature pole (see (33)), we can set $\beta_0 = \infty$ on the right-hand side of (80) so that the trace of the finite-temperature averaged stress tensor is the zero-temperature trace.

This is to be expected. A non-zero trace occurs because of the divergence of quantum field theory which 'cancels off' the zero result expected on the basis of the conformal invariance of the classical theory. Since the divergence is the zerotemperature one, the anomaly will also be that of the zero-temperature theory,

$$g^{\mu\nu}\langle \hat{T}_{\mu\nu}(\mathbf{x})\rangle = \mathbf{i}(\mathbf{x}, t | \boldsymbol{\zeta}(0, \infty) | \mathbf{x}, t).$$
(81)

This is the local form of the anomaly. If x is an interior point of \mathcal{M}_3 the right-hand side is given in terms of the local density $a_2(x, x)$ of the volume part of c_2 (Minak-shisundaram and Pleijel 1949), and so in flat space, for example,

$$g^{\mu\nu}\langle \hat{T}_{\mu\nu}(\boldsymbol{x})\rangle = 0, \qquad \boldsymbol{x} \notin \partial \mathcal{M}_3,$$

However if (81) is integrated over \mathcal{M}_3 we have, in general,

$$\int d\mathbf{x} \, g^{1/2} g^{\mu\nu} \langle \hat{T}_{\mu\nu}(\mathbf{x}) \rangle = -(16\pi^2)^{-1} c_2 \tag{82}$$

with

$$c_2 = a_2 + b_2$$

and even in flat space b_2 is non-zero in general.

Equation (82) can be re-written

$$PV - \frac{1}{3}E = -(48\pi^2)^{-1}c_2 \tag{83}$$

where V is the 'invariant volume' of \mathcal{M}_3 ,

$$V = |\mathcal{M}_3| = \int \mathrm{d}\boldsymbol{x} \, g^{1/2},$$

and P is an 'averaged' pressure

$$P = \frac{1}{3} V^{-1} \int \mathrm{d}\boldsymbol{x} \, g^{1/2} g^{ij} \langle \hat{T}_{ij} \rangle.$$

The operational significance of (81) and (83) is not entirely clear to us.

In d dimensions the local and integrated anomalies are given by $a_{d/2}(x, x)$ and $c_{d/2}(x, x)$ respectively. If d is odd the former vanishes and the latter is a pure boundary term.

8. Conclusion

We wish here only to indicate some open questions and possible extensions.

Clearly it is desirable to discuss the more physical case of electromagnetism (see e.g. Balian and Duplantier 1977) since one has more feeling for the boundary conditions. One could then introduce imperfectly conducting boundaries and it would be very interesting to extend the results of Deutsch and Candelas to determine the form of $\langle \hat{T}_{\mu\nu} \rangle$ near an arbitrarily shaped interface between two dielectrics, at finite temperature.

It is necessary to clear up the possible discrepancy between the local and the global approaches to calculating the total internal energy, say, of the enclosure.

A more exact analysis of the remainder D'_0 terms in the free energy for a general static metric (see equation (52)) is required. It is possible to develop a perturbation method if ∇g_{00} is small (Kennedy, unpublished).

The extension of the theory to conformally static space-times, such as Robertson-Walker universes, is possible and will be dealt with in a further communication.

Finally, the effects of any horizons in \mathcal{M} must be incorporated into the analysis. So far we have ignored these.

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