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Vacuum energy and spectral analysis for Robin boundaries and quantum graphs

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Abstract

In the simplest configurations a solution of a partial differential equation with a Robin boundary condition can be generated from a solution of the corresponding Dirichlet problem. In more general cases similar reasoning can be adapted to construct an approximate solution as a sum over classical paths, which may suffer delayed reflection at the boundary. This analysis provides a new approach to spectral densities and vacuum energy densities. A quantum graph is a network of one-dimensional domains joined at vertices, at which, typically, a close analogue of the Robin boundary condition applies. Our techniques, therefore, apply to such models.

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The research described here has been, or will be, reported in detail in [5, 15, 16]. It stands within the 'classic' paradigm of Casimir calculations. Physical limitations of that paradigm were noted long ago ([10] and related papers by Candelas) and in recent conferences in this series [2, 17]. Such issues are largely irrelevant to the present paper but occasionally need to be recalled to forestall overinterpretation of the mathematical results.

1. The Robin boundary condition

The Robin, or generalized Neumann, condition is

$$\frac{\partial u}{\partial \hat{n}_{\text{in}}} = \alpha u \quad \text{on the boundary } \partial\Omega \tag{1}$$

for a second-order linear partial differential equation in a domain of the form $\Omega \times$ {time interval}, such as

$$\mathrm{i}\frac{\partial u}{\partial t} = Hu, \qquad \frac{\partial^2 u}{\partial t^2} = -Hu, \qquad \ldots. \tag{2}$$

Here H may be the Laplacian $-\nabla^2$ or some more complicated self-adjoint operator. Negative values of α are permissible, but $\alpha(x) \geqslant 0$ is the more physical situation and all that will be treated here.

For example, a one-dimensional wave equation with such a boundary condition describes a vibrating string attached to a discrete massless spring with a Hooke constant α. The energy of such a system is

$$\frac{1}{2}\int_0^L \left[\left(\frac{\partial u}{\partial t}\right)^2 + \left(\frac{\partial u}{\partial x}\right)^2\right] \mathrm{d}x + \frac{\alpha}{2}u(0)^2. \tag{3}$$

The two terms are not separately conserved; the boundary absorbs and emits energy! This fact gives the second-quantized theory a nonlocal character in time that distinguishes Robin boundaries from ordinary Dirichlet and Neumann boundaries.

2. The Dirichlet–Robin transform

The work reported in this section was done in collaboration with a graduate student, Joel Bondurant [5]. The key idea is to invert the operator $T \equiv \frac{\partial}{\partial \hat{n}} - \alpha$ to reduce a Robin problem to a Dirichlet problem. This tactic works perfectly in the easy cases, where T has an obvious extrapolation into the interior of Ω that commutes with H.

More specifically, let us make the *three assumptions* that H has *constant coefficients* and $\alpha = \textit{constant}$ on a *flat* boundary. (Let Ω be the half-space $\{\mathbf{x} \equiv (x, \mathbf{x}_\perp): 0 < x < \infty, \mathbf{x}_\perp \in \mathbf{R}^{d-1}\}$, $\partial\Omega = \{(0, \mathbf{x}_\perp)\}$.) Then, if v solves the Dirichlet problem (for $\frac{\partial^2 u}{\partial t^2} = \pm Hu$ or some such equation)

$$u(\mathbf{x}, t) \equiv T^{-1}v(\mathbf{x}, t) \equiv -\int_0^\infty \mathrm{e}^{-\alpha\epsilon} v(x + \epsilon, \mathbf{x}_\perp, t)\, \mathrm{d}\epsilon \tag{4}$$

solves the corresponding Robin problem. (In fact, it can be defined as the unique solution of slow growth at $x \to +\infty$).

As a corollary, it can be seen that whenever the Dirichlet and Neumann problems can be solved by the textbook method of images

$$G_{\substack{N\\D}}(x, \mathbf{x}_\perp, y, \mathbf{y}_\perp) = G(x - y, \mathbf{x}_\perp - \mathbf{y}_\perp) \pm G(x + y, \mathbf{x}_\perp - \mathbf{y}_\perp), \tag{5}$$

then (because, in operator language, $G_R = T^{-1}G_D T$) the Robin Green function is

$$G_R(x, \mathbf{x}_\perp, y, \mathbf{y}_\perp) = G_N + 2\alpha T_x^{-1} G(x + y, \mathbf{x}_\perp - \mathbf{y}_\perp). \tag{6}$$

This formula enables us to solve all the standard half-space problems with Robin condition. (In the present notation, the condition is

$$\frac{\partial u}{\partial x}(t, 0, \mathbf{x}) = \alpha u(t, 0, \mathbf{x}), \tag{7}$$

which will not be repeated in each example below.)

2.1. Wave equation (spatial dimension 1)

Consider the problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}, \qquad u(0, x) = f(x), \qquad \frac{\partial u}{\partial t}(0, x) = 0. \tag{8}$$

Applying (6) to the well-known d'Alembert solution yields (after discarding terms that vanish for $t > 0$)

$$u(t,x) = \tfrac{1}{2}[f(x-t) + f(x+t) + f(t-x)] - \alpha\theta(t-x)\int_0^{t-x} \mathrm{e}^{-\alpha\epsilon} f(t-x-\epsilon)\,\mathrm{d}\epsilon \tag{9}$$
$$= (\text{Neumann echo}) + (\text{delayed ringing}).$$

2.2. Schrödinger equation (and classical paths)

For

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \nabla_\perp^2 u, \qquad u(0,\mathbf{x}) = f(\mathbf{x}), \tag{10}$$

the method yields

$$G_R = (\text{transverse free propagator})\left\{(\text{Neumann term}) - \frac{2\alpha\sqrt{t}}{\sqrt{4\pi\,\mathrm{i}}}\int_{v_{\min}}^{\infty} \mathrm{e}^{-\alpha u v}\,\mathrm{e}^{\mathrm{i}S}\,\mathrm{d}v\right\}, \tag{11}$$

where v can be identified as the speed of the particle,

$$u \equiv t - \frac{x+y}{v} \tag{12}$$

is the time delay experienced when the particle reflects from the boundary, and

$$S \equiv \tfrac{1}{4}[v(x+y) + v^2 u] \tag{13}$$

has the natural interpretation as the total action of the path (more precisely, of its restriction to the (t,x) plane). For every choice of $(t,\mathbf{x},\mathbf{y})$ there exists (in addition to the direct path) a family of classical trajectories parametrized by v that start at $(0,\mathbf{y})$ and end at $(t,\mathbf{x})$ after a visit to the boundary; $v_{\min} = (x+y)/t$ corresponds to reflection with no delay.

2.3. Heat equation

In this case our main result (and, in a sense, our method) was anticipated in 1891 [7]. Suffice it to say that as a corollary we find the contribution of α (undifferentiated, and not combined with boundary curvature) to the heat-kernel expansion *to all orders*. The results agree with [6, 11], and with [1, 26] where their scopes overlap.

2.4. Vacuum energy

We implement an exponential ultraviolet cutoff by solving

$$\frac{\partial^2 u}{\partial t^2} = -\nabla^2 u, \qquad u(0,\mathbf{x}) = f(\mathbf{x}), \qquad \lim_{t\to+\infty} u(t,\mathbf{x}) = 0. \tag{14}$$

(This is equivalent to inserting the factor $\mathrm{e}^{-t\omega_j}$ into mode sums—integrals in this case.) The *energy density* (for the value $\xi = \frac{1}{4}$ of the conformal coupling) is formally given by

$$T^{00}(x) = -\frac{1}{2}\lim_{t\to 0}\frac{\partial}{\partial t}G_R(t,\mathbf{x},\mathbf{x}). \tag{15}$$

Of course, the limit does not exist; instead, the quantity (15) has a small-t asymptotic expansion including negative powers of t (and sometimes a logarithm). Following standard procedure, we *define* the renormalized energy density as the limit after these divergent terms have been discarded. (For energy densities in locally flat space, the only such term is the ubiquitous zero-point energy of infinite flat space.) In other words, T^{00}_{ren} is the coefficient of the t^1 term in

the small-t expansion of $G_R(t, \mathbf{x}, \mathbf{x})$. It consists of the term that would be present for a pure Neumann boundary plus a Robin correction expressible in terms of the exponential-integral (or incomplete Γ) function. The short-distance behaviour in dimension d is

$$T^{00}_{\text{ren}} \sim O(x^{-(d+1)}) + \alpha O(x^{-d}) + \cdots. \tag{16}$$

The same result was obtained by Romeo and Saharian [25] by a different method (explicit eigenfunctions and modewise vacuum subtraction).

3. More complicated problems; slabs

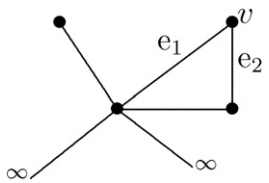
The bad news is that there is no exact, global Dirichlet-to-Robin transform when the *three assumptions* listed above do not hold. (This should be obvious, since $G_R = T^{-1}G_D T$ would imply that the problems had the same spectrum.)

But (as suggested by the structure of the foregoing examples) we can hope to exploit the locality of the interaction to construct an approximate, infinite-series solution as a *sum over classical paths*. The example worked out in [5] is the wave equation on an interval with a Robin boundary at the left and a Dirichlet boundary at the right. It proved possible to evaluate in a closed form the integrals over the exponential delay tails at the Robin end, repeatedly compounded by multiple reflections.

In [5] we did not consider vacuum energy for the finite interval, but currently another graduate student, Zhonghai Liu, and I are calculating the vacuum energy (and energy density) in a slab of arbitrary dimension with at least one Robin boundary surface [16]. The multiple-reflection analysis continues to apply. The case with one Robin and one Dirichlet 'plate' is nearly completed. For the energy density (with $\xi = \frac{1}{4}$), we have verified that the periodic paths give a spatially constant Casimir energy, while the bounce paths (closed but not periodic) produce the behaviour (16) at each end, as expected (for example, from the classic work of Deutsch and Candelas [10]). On the finite interval, one can (and we shall) apply the same cutoff and renormalization procedure to the *total energy*, obtaining (by definition) a finite result of the sort expected from the similar literature [4, 13, 14, 18]. (It is notorious that this renormalized total energy is not the spatial integral of the renormalized density, which is infinite. Presumably, the fault is on both sides: the singularities in the density would go away if the idealized boundary were replaced by a realistic model of a material with atomic structure, and some of the cutoff-dependent terms in the total energy, rather than being thrown away, should be absorbed into (nonzero and possibly large) terms describing the boundary material itself.) When our work is complete, the results will presumably agree with those of [25] but will be independent of them (being path sums, not (complicated) integral formulae).

4. Quantum graphs

A quantum graph combines the features of one-dimensional and multi-dimensional systems. It is a system of vertices with attached edges, some of which may extend to infinity:



(17)

On each edge the free Schrödinger equation holds,

$$-\frac{\mathrm{d}^2}{\mathrm{d}x_\mathrm{e}^2}u = \omega^2 u. \tag{18}$$

At each vertex, u is continuous and a generalized Kirchhoff condition holds,

$$\sum_\mathrm{e} \frac{\mathrm{d}u}{\mathrm{d}x_\mathrm{e}} = \alpha u(v). \tag{19}$$

(This is a somewhat restricted definition of 'quantum graph'. Other edge operators and other vertex boundary conditions are also studied in the literature.)

Note that a quantum graph is a *metric graph*, not a *combinatorial graph* where the edges are inert and the Hamiltonian is a discrete Laplacian acting on the vertices [8]:

$$\Delta u(v) \equiv (\mathrm{const})u(v) - \sum_{\text{neighbours}} u(v_n). \tag{20}$$

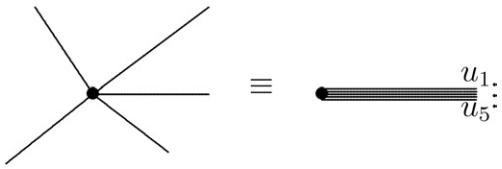
Quantum graphs are the focus of growing interest [19–23]. They have applications in modelling thin three-dimensional structures (quantum wires) [21]; in symbolic dynamics for wave propagation in piecewise homogeneous media [9]; in modelling lungs, veins, etc (see various papers presented at the Snowbird conference [3]). Finally, they show some promise in modelling multi-dimensional (continuum) quantum-mechanical systems [24, 12]. A linear quantum graph

(21)

is equivalent to the one-dimensional Schrödinger equation with $V(x) = \alpha \sum_j \delta(x - j)$. Higher dimensions can be partially discretized by, e.g., a rectangular grid.

4.1. An infinite star graph

Take a graph with one vertex and N infinite edges, and bundle all its edges together:



(22)

Its Schrödinger equation is clearly equivalent to that for a multicomponent wavefunction defined on a half-line,

$$u = \{u_j(x)\} \in L^2(0, \infty)^N. \tag{23}$$

Here, the Hamiltonian is just $H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the boundary conditions

$$u_j(0) = u(0) \quad \text{(i.e., is independent of } j\text{)}, \tag{24}$$

$$\sum_{j=1}^N u_j'(0) = \alpha u(0). \tag{25}$$

The old Robin problem of previous sections is just this with $N = 1$.

In analogy with those sections, one finds [15] the Dirichlet-to-Robin formulae

$$(T^{-1}v)_j(x) = \frac{1}{\alpha}\left[\frac{1}{N}\sum_{k=1}^N v_k(x) - v_j(x)\right] - \frac{1}{N^2}\int_x^\infty \mathrm{e}^{-\alpha(s-x)/N}\sum_{k=1}^N v_k(s)\,\mathrm{d}s, \tag{26}$$

$$G_{Sj}{}^{l}(t,x,y) = \delta_j^l G(t,|x-y|) + \left(\frac{2}{N} - \delta_j^l\right) G(t,x+y) - \frac{2\alpha}{N^2}\int_0^\infty \mathrm{e}^{-\alpha(s-x)/N} G(t,s+y)\,\mathrm{d}s. \tag{27}$$

Here $G_{Sj}{}^{l}$ is the matrix Green function on the graph, and $G(t,z)$ is the corresponding (scalar) Green function on the real line.

4.2. Vacuum energy on a quantum graph

Here we study the graph as an abstract bosonic system, with no pretensions to modelling a structure in a three-dimensional space. For the vacuum energy problem $\left(\frac{\partial^2 u}{\partial t^2} + \frac{\partial^2 u}{\partial x^2} = 0\right)$, one has

$$G(t,z) = \frac{t/\pi}{t^2+z^2}, \tag{28}$$

and hence from (27)

$$G_{Sj}{}^{l} = \delta_j^l \frac{t/\pi}{t^2+(x-y)^2} + \left(\frac{2}{N} - \delta_j^l\right)\frac{t/\pi}{t^2+(x+y)^2} + \frac{2\alpha}{\pi N^2}\,\mathrm{e}^{\alpha(x+y)/N}\,\mathrm{Im}\left[\mathrm{e}^{-\mathrm{i}\alpha t/N}\,\mathrm{Ei}\left(\frac{\mathrm{i}\alpha t}{N} - \frac{\alpha}{N}(x+y)\right)\right]. \tag{29}$$

Proceeding from (15) as before, we obtain [15]

$$T_{\mathrm{ren}}^{00}(x) = \left(1-\frac{2}{N}\right)\frac{1}{8\pi x^2} + \frac{\alpha}{2\pi N^2 x} + \frac{\alpha^2}{\pi N^3}\,\mathrm{e}^{2\alpha x/N}\,\mathrm{Ei}\left(-\frac{2\alpha x}{N}\right). \tag{30}$$

An instructive alternative calculation uses $G_{Sj}{}^{l}$ for the *wave* equation to find (as its inverse cosine transform) the *local spectral density*

$$\rho_{Sj}{}^{j}(\omega,x,x) = \frac{1}{\pi} + \frac{1}{\pi}\left(\frac{2}{N}-1\right)\cos(2\omega x) + \frac{2\alpha/\pi}{\alpha^2+N^2\omega^2}\left[\omega\sin(2\omega x) - \frac{\alpha}{N}\cos(2\omega x)\right]. \tag{31}$$

Then we can compute the 'mode sum' for T_{ren}^{00} from

$$\rho_{Sj}{}^{j}(\omega,x,x) - \frac{1}{\pi}. \tag{32}$$

The results are consistent, of course.

Finally, let us examine the formulae for their physical significance (within the model). In the infinite star graph one sees only boundary effects. At short distance, the Kirchhoff (i.e., $\alpha = 0$, $\sum u_j'(0) = 0$) term dominates:

$$T^{00}(x) \sim \left(1-\frac{2}{N}\right)\frac{1}{8\pi x^2} + \frac{\alpha}{2\pi N^2 x} + \frac{\alpha^2}{\pi N^3}\ln|\alpha x| + O(\alpha^2 x^2). \tag{33}$$

At large distance, the energy density is almost pure Dirichlet (by which one means the case $\alpha \to +\infty$, $u_j(0) = 0$ for all j),

$$T^{00}(x) \sim \frac{1}{8\pi x^2} + O(\alpha^{-1}x^{-3}). \tag{34}$$

True Casimir energies will appear when a *finite* star graph is studied.

Acknowledgments

In addition to the two students, I thank Peter Kuchment and his young colleagues for initiating me into the quantum graph fraternity—in particular, inviting me to participate in the Snowbird conference [3] in the faith that I would for the first time do some research in the subject.

Note added in proof. Earlier work on vacuum energy with a Robin boundary was done by S L Lebedev 1996 *Zh. Eksp. Teor. Fiz.* **110** 769–92 [1996 *JETP* **83** 423–34] and 2001 *Yad. Fiz.* **64** 1413–22 [2001 *Phys. Atomic Nuclei* **64** 1337–46].

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