The Boundary-Integral Formulation and Multiple-Reflection Expansion for the Vacuum Energy of Quantum Graphs

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Abstract. Vacuum energy and other spectral functions of Laplace-type differential operators have been studied approximately by classical-path constructions and more fundamentally by boundary integral equations. As the first step in a program of elucidating the connections between these approaches and improving the resulting calculations, I show here how the known solutions for Kirchhoff quantum graphs emerge in a boundary-integral formulation.

PACS numbers: 02.60.Lj, 11.10.Kk, 42.25.Gy

AMS classification scheme numbers: Primary 34B45; Secondary 34B27, 81Q20
1. Introduction

1.1. Vacuum energy density and cylinder kernels

The energy density of a quantum field in its vacuum state (or a state of fixed temperature), given particular time-independent external conditions, is of interest in cosmology, hadronic physics, and soft condensed matter physics (where the fluctuations involved are of thermal rather than quantum origin). Most famously, electromagnetic vacuum energy gives rise to the observed Casimir force between conducting bodies (and its counterpart for dielectrics, the Lifshitz force).‡ The study of gravitational effects (or their negligibility, even in the presence of divergences) requires detailed knowledge of all components of the stress-energy-momentum tensor of the field as functions of position in space. This local information is also helpful in addressing such subjects of continued investigation and debate as the occasionally counterintuitive signs of the calculated forces, and the meaning of the divergences resulting from idealized boundary conditions.

A convenient way to study vacuum energy is to insert (usually temporarily) an exponential ultraviolet cutoff in the spectral expansions of the stress tensor or the total energy. For the fiducial toy model, a scalar field, this procedure leads quickly to the study of the cylinder (or Poisson) kernels, which are Green functions for certain elliptic boundary value problems in one higher spatial dimension [23, 5, 10]. In cavities or billiards the cylinder kernel lends itself to the same kind of semiclassical or optical expansion that is more often (e.g., [29]) applied to the Green functions for the heat, Schrödinger, or resolvent kernels. (I hope to publish elsewhere a detailed justification and development of this assertion.) For rectangular cavities this construction reduces to the classic “method of images” and yields exact results [11, 21], revealing, for example, that the divergent pressure on one face of a rectangle is related to the divergent energy density parallel to the adjacent faces. This insight is clearly pertinent to the vexed question of the vacuum pressure on a conducting sphere, where perpendicular boundary surfaces do not exist. Unfortunately, in the presence of curved surfaces (or, a fortiori, edges and corners) the optical construction is no longer exact. Preliminary calculations show that the leading semiclassical approximation is not adequate to understand the radial pressure in a sphere, and that in problems with curved boundaries the construction of higher-order approximations is blocked by problems of the same type that arose in connection with the heat kernel [25, 24]. When the boundary is not smooth, the leading optical approximation is completely unacceptable until supplemented by diffractive contributions (e.g., [17, 7]), which are hard to calculate in generality.

‡ In lieu of a long list of references on vacuum energy, I recommend the recent special issues of New Journal of Physics [33] and Journal of Physics A [34] and the bibliographies of the papers therein.
1.2. Boundary integrals and multiple reflection

Although higher-order optical approximations for smooth curved boundaries and diffractive approximations for nonsmooth ones can sometimes be found by trial and error and verified \textit{a posteriori}, a more systematic approach is desirable. In principle, such an approach is available in the standard mathematical literature on partial differential and integral equations \cite{22, 30, 31, 8, 28}. A partial differential equation with boundary conditions can be reduced to an integral equation on the boundary. Up to some convergence issues touched upon lightly in Appendix B, the solution of the integral equation by the methods of Volterra or Fredholm is constructive. The result is a \textit{multiple reflection expansion} (MRE) expressing the Green function of the original problem as a series \( \sum_{N=0}^{\infty} G_N \), where \( G_N \) is an \( N \)-fold integral over the boundary; the solution is formally a “sum” over all paths from the source point to the field point, each path bouncing off the boundary \( N \) times (in general nonspecularly). This construction was famously applied to physical problems by Balian and Bloch \cite{1, 2, 3}. (See also \cite{26} in the case of the heat equation.) The more familiar (and simpler) semiclassical or optical approximations (involving only specular reflections) for the heat, Schrödinger, and resolvent equations emerge from the MRE when the integrals are approximated by steepest descent or stationary phase. In the case of the cylinder kernel treated directly by MRE, the appropriate approximation method is not so obvious; cylinder kernels can also be obtained from the other kernels by integral transformations, but at the cost of integrating parameters over values where the validity of the (e.g.) stationary-phase approximation is dubious. This circumstance calls for a careful examination of the implications of the MRE for the representation and approximation of cylinder kernels for curved or nonsmooth boundaries — and, indeed, at the first step, even for flat smooth boundaries.

1.3. Quantum graphs

The present paper is a preliminary foray with primarily pedagogical intent. The application of the MRE to vacuum energy needs to be studied first in the simplest case, one spatial dimension. But a one-dimensional cavity is just an interval, too trivial to occupy one’s attention for long. A generalization, which combines the ease of exact solution of a one-dimensional problem with some of the nontrivial properties of multidimensional systems, is the concept of a quantum graph.

A \textit{quantum graph} \cite{20, 15} is a Riemannian one-complex — that is, a network of edges and vertices equipped with a natural notion of arc length on each edge. There follows a natural definition of the Laplacian operator as \( d^2/dx^2 \) on each edge, supplemented by boundary conditions at each vertex to make the operator self-adjoint. In particular, the most natural and popular boundary conditions are the \textit{Kirchhoff conditions}: Functions in the domain of the operator are required to be continuous at the vertices, while the outward derivatives of a function on all the edges incident on a given vertex are required to sum to zero. (A vertex attached to only one edge is thus a Neumann endpoint in the
On a Kirchhoff quantum graph the semiclassical approximation again reduces to the (exact) method of images, which is, nevertheless, quite intricate to execute. Solutions for the heat and resolvent equations have been known for some time \cite{27, 19, 4, 18}. The corresponding construction for the cylinder kernel has been extensively investigated by Wilson et al. \cite{32, 12, 13, 14, 6}. Here I show how the same results can be obtained from an MRE, temporarily ignoring the fact that the simpler ansatz is already exact. The connection is not exactly trivial, so the exercise will be useful in tackling more serious models later. (It also enables us to get out of the way some complications peculiar to the one-dimensional case, associated with the logarithmic form of the integral kernel \cite{11}.)

Section 2 sets up some machinery. The next four sections consider four increasingly complicated scenarios: an interval with one endpoint, a graph with one vertex but arbitrarily many edges, an interval with two endpoints, and finally a general quantum graph (with finitely many edges, finite in length). In each case the MRE calculations are carried only to the point where it is obvious how to continue them and match them up with known results. The main point becomes visible in the third case (section 5), where a nontrivial boundary integral equation must be derived and iteratively solved for the first time. Some necessary integrals are evaluated in Appendix A. Of greater interest is Appendix B, where the mathematical status of the multiple-reflection series is discussed, and the possible utility of the exact Fredholm solution in the situation of finite temperature is pointed out. The machinery for finite temperature is set up in Appendix C.

2. Notation

Let $\Gamma$ be a quantum graph, and let $\tilde{\Gamma} = \mathbb{R} \times \Gamma$ be the corresponding “Euclideanized space-time”. Variables $x, y, \ldots$ stand for points in $\Gamma$ and variables $s, t, \ldots$ for real numbers. I consider here only the standard Kirchhoff boundary conditions.

The Green function for the Poisson equation in $\mathbb{R}^2$ is

$$G_0(t, x; s, y) = -\frac{1}{2\pi} \ln \left( \frac{r}{r_0} \right)$$

$$= -\frac{1}{4\pi} \ln[(t - s)^2 + (x - y)^2] + C.$$  \hspace{1cm} (1)

Let $G(t, x; s, y)$ be the Green function for the Poisson equation in $\tilde{\Gamma}$. Then the cylinder kernels in $\tilde{\Gamma}$ are

$$\overline{T}(t, x, y) = -2G(t, x; 0, y),$$  \hspace{1cm} (2)

$$T(t, x, y) = -2 \frac{\partial G}{\partial t}(t, x; 0, y).$$  \hspace{1cm} (3)

$G_0$ is defined only modulo the indicated scale ambiguity (the arbitrary constants $r_0$ and $C$), but $T_0$ and the spatial derivatives of $G_0$ are unique. Henceforth we take $C = 0$. 
For later use note
\[
\frac{\partial G_0(t, x; s, y)}{\partial x} = -\frac{1}{2\pi} \frac{x - y}{(t - s)^2 + (x - y)^2} = -\frac{\partial G_0}{\partial y}. \tag{4}
\]
Related to this function is the well known distributional identity
\[
\lim_{x \to 0} \frac{1}{\pi} \frac{x}{(t - s)^2 + x^2} = \delta(t - s), \tag{5}
\]
which will be used repeatedly in what follows.

3. Case 1: \( \Gamma = \mathbb{R}^+ \)

We will solve the Poisson equation on the half-plane with Neumann boundary at \( y = 0 \).

Make the ansatz
\[
G = G_0 + \gamma, \tag{6}
\]
\[
\gamma(t, x; s_0, y_0) = \int_{-\infty}^{\infty} ds G_0(t, x; s, 0) \mu_0(s), \tag{7}
\]
where \( \mu_0 \) has a dependence on \((s_0, y_0)\) that will be notationally suppressed. The integral
in (7) is over the boundary \( \{(s, y): y = 0\} \), and the subscript on \( \mu \) refers to that value of \( y \).

We calculate from (4)
\[
\frac{\partial \gamma}{\partial x}(t, 0; s_0, y_0) = -\int_{-\infty}^{\infty} ds \frac{x - y}{2\pi} \left[ \frac{(t - s)^2 + (x - y)^2}{2\pi} \right]^{-1} \bigg|_{x=y=0} \mu_0(s)
= 0. \tag{8}
\]
As always in the boundary-integral method, we must make a careful distinction between the value of such an integral exactly on the boundary \((x = 0)\) and the limit of the integral as the boundary is approached from the interior. For the latter we have by (4) and (5)
\[
\frac{\partial \gamma}{\partial x}(t, x; s_0, y_0) = -\int_{-\infty}^{\infty} ds \frac{x}{2\pi} \left[ \frac{(t - s)^2 + x^2}{2\pi} \right]^{-1} \mu_0(s)
\to -\frac{1}{2} \mu_0(t) \quad \text{as} \; x \downarrow 0, \tag{9}
\]
and it is this object that must be chosen to satisfy the Neumann boundary condition:
\[
0 = \frac{\partial G}{\partial x}(t, 0^+; s_0, y_0) = \frac{\partial G_0}{\partial x} + \frac{\partial \gamma}{\partial x}
\]
implies
\[
\mu_0(t) = 2 \frac{\partial G_0}{\partial x}(t, 0^+; s_0, y_0) = \frac{y_0}{\pi} \left[ \frac{(t - s_0)^2 + y_0^2}{(t - s_0)^2 + y_0^2} \right]^{-1} \tag{10}
\]
and hence
\[
\gamma(t, x; s_0, y_0) = -\frac{y_0}{4\pi^2} \int_{-\infty}^{\infty} ds \ln\left[ \frac{(t - s)^2 + x^2}{(t - s_0)^2 + y_0^2} \right]^{-1}. \tag{11}
\]
But from the method of images we know a more elementary formula for \( \gamma \):
\[
\gamma(t, x; s_0, y_0) = G_0(t, x; s_0, -y_0) = -\frac{1}{4\pi} \ln\left[ \frac{(t - s_0)^2 + (x + y_0)^2}{(t - s_0)^2 + (x - y_0)^2} \right]. \tag{12}
\]
The equivalence of (11) and (12) is shown in Appendix A.
4. Case 2: Infinite star graphs

Let \( d_v \) be the number of edges meeting at the central vertex. On edge \( j \) there is a coordinate \( x_j \), sometimes written \( x_j \), equal to 0 at the vertex. Without loss of generality we can take \( y_0 \) to be located on edge \( j = 1 \).

In analogy with (6) and (7) we construct the Green function in the form

\[
G_j = \begin{cases} 
G_0 + \gamma_j & \text{if } j = 1, \\
\gamma_j & \text{if } j \neq 1,
\end{cases}
\]

\[
\gamma_j(t, x; s_0, y_0) = \int_{-\infty}^{\infty} ds G_0(t, x; s, 0) \mu_j(s) + \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial y}(t, x; s, 0) \nu_j(s) \\
= -\frac{1}{4\pi} \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + x^2] \mu_j(s) \\
+ \frac{x}{2\pi} \int_{-\infty}^{\infty} ds [(t - s)^2 + x^2]^{-1} \nu_j(s).
\]

(Here the dependence of \( \mu \) and \( \nu \) on the vertex \( v \) is suppressed, along with that on \((s_0, y_0)\).)

The Kirchhoff boundary conditions are

\[ G_j(t, 0; s_0, y_0) = G_k(t, 0; s_0, y_0) \quad \text{for all } j, k, \]

\[ \sum_{j=1}^{d_v} \frac{\partial G_j}{\partial x}(t, 0; s_0, y_0) = 0. \]

They translate into

\[ \gamma_j(t, 0^+; s_0, y_0) = \gamma_k(t, 0^+; s_0, y_0) \quad \text{for all } j, k \neq 1, \]

\[ \gamma_1(t, 0^+; s_0, y_0) = \gamma_k(t, 0^+; s_0, y_0) - G_0(t, 0; s_0, y_0) \quad \text{(for any } k \neq 1), \]

\[ \sum_{j=1}^{d_v} \frac{\partial \gamma_j}{\partial x}(t, 0^+; s_0, y_0) = -\frac{\partial G_0}{\partial x}(t, 0; s_0, y_0). \]

The symmetries of these equations suggest the further ansätze

All \( \mu_j \) are equal,

All \( \nu_j \) are equal except \( \nu_1 \),

\[ \sum_{j=1}^{d_v} \nu_j = 0. \]

Then (17) is satisfied, and (18) becomes, by analogy with (9),

\[ \nu_1(t) - \nu_k(t) = -2G_0(t, 0; s_0, y_0) = \frac{1}{2\pi} \ln[(t - s_0)^2 + y_0^2]. \]

Sum (23) over all \( k \neq 1 \) and use (22):

\[ \frac{d_v}{2\pi} \ln[(t - s_0)^2 + y_0^2] = (d_v - 1)\nu_1 - \sum_{k \neq 1} \nu_k = d_v\nu_1 - \sum_{j=1}^{d_v} \nu_j = d_v\nu_1. \]
Thus
\[ \nu_1(t) = \left(1 - \frac{1}{d_v}\right) \frac{1}{2\pi} \ln[(t - s_0)^2 + y_0^2], \] (24)
and then
\[ \nu_k(t) = -\frac{1}{2\pi d_v} \ln[(t - s_0)^2 + y_0^2]. \] (25)

Finally, to impose (19) and find \( \mu_j \) we note from (14) that
\[ \frac{\partial \gamma_j}{\partial x}(t, x; s_0, y_0) = -\frac{x}{2\pi} \int_{-\infty}^{\infty} ds \left[ (t - s)^2 + x^2 \right]^{-1} \mu_j(s) + \int_{-\infty}^{\infty} ds \frac{\partial^2 G_0}{\partial x \partial y}(t, x; s, 0) \nu_j(s), \]
and hence from (19) and (22)
\[ -\frac{\partial G_0}{\partial x}(t, 0; s_0, y_0) = -\lim_{x \rightarrow 0} x \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \left[ (t - s)^2 + x^2 \right]^{-1} \sum_{j=1}^{d_v} \mu_j(s). \]

It follows by (20), (11), and (5) that
\[ \mu_j(t) = \frac{y_0}{\pi d_v} \left[ (t - s_0)^2 + y_0^2 \right]^{-1}. \] (26)

Inserting (24)–(26) into (14) we arrive at
\[ \gamma_j(t, x; s_0, y_0) = -\frac{1}{4\pi^2 d_v} \int_{-\infty}^{\infty} ds y_0 \frac{\ln[(t - s)^2 + x^2]}{(s - s_0)^2 + y_0^2} \]
\[ + \left( \delta_{1j} - \frac{1}{d_v} \right) \frac{1}{4\pi^2} \int_{-\infty}^{\infty} ds x \frac{\ln[(s - s_0)^2 + y_0^2]}{(t - s)^2 + x^2}. \] (27)

The two integrals in (27) are identical except for the interchange \((t, x) \leftrightarrow (s_0, y_0)\). Moreover, at the end of the previous section, and in (A.3), we observed that
\[ \frac{y_0}{\pi} \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + x^2][(s - s_0)^2 + y_0^2] = \ln[(t - s_0)^2 + (x + y_0)^2]; \] (28)
this function is actually invariant under that interchange. (In (28) it is assumed that \( x \) and \( y_0 \) are positive.) So we finally arrive at
\[ \gamma_j(t, x; s_0, y_0) = \left( \delta_{1j} - \frac{2}{d_v} \right) \frac{1}{4\pi} \ln[(t - s_0)^2 + (x + y_0)^2], \] (29)
where we now allow for \( y_0 \) to be located on any edge, \( l \). This is equivalent to known results for quantum star graphs (e.g., [19, Sec. 3B], [32, Ch. 3]). From (3), the formula for the cylinder kernel \( T \) is
\[ T_j^l(t, x, y) = \delta_j^l \frac{t/\pi}{t^2 + (x - y)^2} + \left( \frac{2}{d_v} - \delta_j^l \right) \frac{t/\pi}{t^2 + (x + y)^2}, \] (30)
which is equation (35) of [9] with the Robin parameter \( \alpha = 0 \).
5. **Case 3:** $\Gamma = (0, L)$

I write $\partial/\partial n$ for an *inward* normal derivative in the usual sense of bounded domains. In the graph context such a derivative is *outward* from a vertex.

In the present model the boundary has two parts, $\{(s, y) : y = 0\}$ and $\{(s, y) : y = L\}$, the boundary condition is still Neumann, and the obvious ansatz is (6) with

$$\gamma(t, x; s_0, y_0) = \int_{-\infty}^{\infty} ds \, G_0(t, x, s) \mu_0(s) + \int_{-\infty}^{\infty} ds \, G_0(t, x, L) \mu_L(s).$$  \hspace{1cm} (31)

Evaluate the derivative:

$$\frac{\partial \gamma}{\partial x}(t, x; s_0, y_0) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} ds \frac{x}{(t-s)^2 + x^2} \mu_0(s)$$

$$- \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \frac{x - L}{(t-s)^2 + (x-L)^2} \mu_L(s).$$ \hspace{1cm} (32)

The limits of the normal derivatives from inside are

$$\frac{\partial \gamma}{\partial n}(0^+) \equiv \frac{\partial \gamma}{\partial x}(t, 0^+; s_0, y_0) = - \frac{1}{2} \mu_0(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \frac{L}{(t-s)^2 + L^2} \mu_L(s),$$ \hspace{1cm} (33)

$$\frac{\partial \gamma}{\partial n}(L^-) \equiv - \frac{\partial \gamma}{\partial x}(t, L^-; s_0, y_0) = - \frac{1}{2} \mu_L(t) + \frac{1}{2\pi} \int_{-\infty}^{\infty} ds \frac{L}{(t-s)^2 + L^2} \mu_0(s).$$ \hspace{1cm} (34)

(The sign constraint in (9) becomes $L-x \downarrow 0$ in going from (32) to (34).) The appropriate boundary conditions are

$$\frac{\partial \gamma}{\partial n}(0^+) = - \frac{\partial G_0}{\partial x}(t, 0; s_0, y_0), \quad \frac{\partial \gamma}{\partial n}(L^-) = + \frac{\partial G_0}{\partial x}(t, L; s_0, y_0).$$ \hspace{1cm} (35)

From these relations we obtain the basic boundary-integral equations of the problem,

$$\mu_0(t) = \frac{1}{\pi} \frac{y_0}{(t-s_0)^2 + y_0^2} + \frac{1}{\pi} \int_{-\infty}^{\infty} ds \frac{L}{(t-s)^2 + L^2} \mu_L(s),$$

$$\mu_L(t) = \frac{1}{\pi} \frac{L - y_0}{(t-s_0)^2 + (L-y_0)^2} + \frac{1}{\pi} \int_{-\infty}^{\infty} ds \frac{L}{(t-s)^2 + L^2} \mu_0(s).$$ \hspace{1cm} (36)

More abstractly, the system (36) is

$$\mu_\nu(t) = \frac{1}{\pi} \frac{d(v, y_0)}{(t-s_0)^2 + d(v, y_0)^2} + \frac{1}{\pi} \int_{-\infty}^{\infty} ds \frac{L}{(t-s)^2 + L^2} \mu_\nu(s),$$ \hspace{1cm} (37)

where $d(v, y_0)$ is the distance from vertex $v$ to $y_0$, and $\nu$ is the *other* vertex. Still more abstractly, fix a vertex $v_*$; then

$$\mu_{v_*}(t) = 2 \frac{\partial G_0}{\partial n}(t, v_*; s_0, y_0) + 2 \int_{\partial \gamma} \frac{\partial G_0}{\partial n}(t, v_*; s, v) \mu_\nu(s),$$ \hspace{1cm} (38)

where a sum over $\nu$ is implicit in the integration over the total boundary $\partial \Gamma = \mathbf{R} \times \partial \Gamma$ of the graph, and it happens, as in (8), that

$$\frac{\partial G_0}{\partial n}(t, v_*; s, v_*) = 0.$$ \hspace{1cm} (39)

Even more abstractly, the integral equation has the form

$$\mu = g_0 + K\mu,$$ \hspace{1cm} (40)
so that formally

\[
\mu = (1 - K)^{-1}g_0 \sim (1 + K + K^2 + \cdots)g_0.
\]  

(41)

Postponing to Appendix B the issue of the convergence of the Neumann series \((41)\), we examine its zeroth term, which produces the first-order (not leading) term in the series for \(G\). That is, one drops the integrals in \((36)\) and substitutes \((36)\) into \((6)\) and \((31)\):

\[
G(t, x; s_0, y_0) = G_0(t, x; s_0, y_0)
\]

\[
- \frac{1}{4\pi^2} \left\{ \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + x^2] \frac{y_0}{(t - s)^2 + y_0^2} + \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + (L - x)^2] \frac{L - y_0}{(t - s)^2 + (L - y_0)^2} \right\}
\]

\[
= - \frac{1}{4\pi} \left\{ \ln[(t - s_0)^2 + (x + y_0)^2] + \ln[(t - s_0)^2 + (2L - x - y_0)^2] \right\},
\]  

(42)

where \((28)\) has been used (with \(L - x > 0, L - y_0 > 0\)). Clearly, \((42)\) comprises the single-reflection terms in the standard solution by the method of images (images at \(-y_0\) and \(2L - y_0\)).

The first-order term in \((41)\) should therefore yield the two-reflection terms in the image solution. Substituting the zeroth-order \(\mu\) (the first terms in \((36)\)) into the integrals in \((36)\), one gets

\[
\mu_0(t) - \frac{1}{\pi} \frac{y_0}{(t - s_0)^2 + y_0^2} = \frac{1}{\pi^2} \int_{-\infty}^{\infty} ds \frac{L(L - y_0)}{[(t - s)^2 + L^2][(s - s_0)^2 + (L - y_0)^2]}
\]

\[
= \frac{1}{\pi} \frac{L(L - y_0)}{(t - s_0)^2 + (L - y_0)^2},
\]

\[
\mu_L(t) - \frac{1}{\pi} \frac{L - y_0}{(t - s_0)^2 + (L - y_0)^2} = \frac{1}{\pi^2} \int_{-\infty}^{\infty} ds \frac{L y_0}{[(t - s)^2 + L^2][(s - s_0)^2 + y_0^2]}
\]

\[
= \frac{1}{\pi} \frac{L y_0}{(t - s_0)^2 + (L + y_0)^2}.
\]  

(43)

(For the evaluation of these integrals see \((A.1)\).) The resulting additional terms in \(G\) are

\[
- \frac{1}{4\pi^2} \left\{ \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + x^2] \frac{2L - y_0}{(s - s_0)^2 + (2L - y_0)^2} + \int_{-\infty}^{\infty} ds \ln[(t - s)^2 + (L - x)^2] \frac{L + y_0}{(s - s_0)^2 + (L + y_0)^2} \right\}
\]

\[
= - \frac{1}{4\pi} \left\{ \ln[(t - s_0)^2 + (x + 2L - y_0)^2] + \ln[(t - s_0)^2 + (2L - x + y_0)^2] \right\}.
\]  

(44)

Exactly as expected, these terms describe images at \(y_0 - 2L\) and \(y_0 + 2L\).

6. Case 4: General compact Kirchhoff quantum graphs

Notation: \(v\) is a vertex of degree \(d_v\); \(e\) is an edge. Whenever considering a fixed vertex \(v\), we can assume that the edges are parametrized so that \(x \equiv x_e = 0\) at \(v\); each incident
edge \((e \in E_v)\) will then have a terminal vertex \(t_e\) at which \(x_e = L_e\). Let \(e_0\) be the edge containing the source point \(y_0\).

**Ansatz** (generalizing (14) and (31)):

\[
G_e = \delta_{e0} G_0 + \gamma_e. \tag{45}
\]

For every \(v\) and every \(e \in E_v\) there will be charge and dipole densities \(\mu_{ev}(t)\) and \(\nu_{ev}(t)\) (with hidden dependence on \((s_0, y_0)\) as usual). For temporary notational purposes, given \(e\) choose one of its two vertices, \(v\), as its initial vertex. Then

\[
\gamma_e(t, x; s_0, y_0) = \int_{-\infty}^{\infty} ds \, G_0(t, x; s, 0) \mu_{ev}(s) + \int_{-\infty}^{\infty} ds \, G_0(t, x; s, L_e) \mu_{et}(s)
+ \int_{-\infty}^{\infty} ds \, \frac{\partial G_0}{\partial y}(t, x; s, 0) \nu_{ev}(s) - \int_{-\infty}^{\infty} ds \, \frac{\partial G_0}{\partial y}(t, x; s, L_e) \nu_{et}(s). \tag{46}
\]

**Boundary conditions:** Also for temporary purposes, consider a fixed \(v\) and assume the edges in \(E_v\) are numbered \(1, \ldots, d_v\). (Of course, this list may or may not include \(e_0\).) Then the boundary conditions at \(v\) are, for all \(e\) and \(f\) in \(E_v\),

\[
\gamma_e(t, 0; s_0, y_0) + \delta_{e0} G_0(t, 0; s_0, y_0) = \gamma_f(t, 0; s_0, y_0) + \delta_{f0} G_0(t, 0; s_0, y_0), \tag{47}
\]

\[
\sum_{e=1}^{d_v} \frac{\partial \gamma_e}{\partial x}(t, 0; s_0, y_0) = -\frac{\partial G_0}{\partial x}(t, 0; s_0, y_0) \sum_{e=1}^{d_v} \delta_{e0}. \tag{48}
\]

For (48) we calculate

\[
\frac{\partial \gamma_e}{\partial x}(t, x; s_0, y_0) = \int_{-\infty}^{\infty} ds \, \frac{\partial G_0}{\partial x}(t, x; s, 0) \mu_{ev}(s) + \int_{-\infty}^{\infty} ds \, \frac{\partial G_0}{\partial x}(t, x; s, L_e) \mu_{et}(s)
+ \int_{-\infty}^{\infty} ds \, \frac{\partial^2 G_0}{\partial x \partial y}(t, x; s, 0) \nu_{ev}(s) - \int_{-\infty}^{\infty} ds \, \frac{\partial^2 G_0}{\partial x \partial y}(t, x; s, L_e) \nu_{et}(s). \tag{49}
\]

**Integral equation system:** Of the three simplifying symmetry relations (20)–(22), the first and third are fundamental (essentially characterizing the solutions for the Dirichlet and Neumann subspaces of the graph — see, e.g., [20, 13]). They can immediately be generalized to the present situation:

\[
\mu_{ev} = \mu_{fv} \quad \text{for all } e, f \in E_v, \tag{50}
\]

\[
\sum_{e=1}^{d_v} \nu_{ev} = 0. \tag{51}
\]

However, (21) was a symmetry that may no longer hold, because even if \(y_0\) does not fall on any \(e \in E_v\), some of those edges are “closer” to \(y_0\) than others. As before, (50) and (51) assure that all nontrivial integrals at \(v\) in (46)–(48) cancel. They also reduce the number of unknowns from \(2d_v\) to \(d_v\), which is the number of independent equations in (47) and (48). For the trivial integrals we have as usual

\[
\frac{\partial G_0}{\partial x}(t, x; s, 0) = -\frac{x-0}{2\pi \left[(t-s)^2 + (x-0)^2\right]} \rightarrow -\frac{1}{2} \delta(t-s) \quad \text{as } x \downarrow 0. \tag{52}
\]

Thus (47) reduces to

\[
\frac{1}{2} \nu_{ev}(t) + \int_{-\infty}^{\infty} ds \, G_0(t, 0; s, L_e) \mu_{et}(s) - \int_{-\infty}^{\infty} ds \, \frac{\partial G_0}{\partial y}(t, 0; s, L_e) \nu_{et}(s) + \delta_{e0} G_0(t, 0; s_0, y_0)
= \text{same with } e \rightarrow f. \tag{53}
\]
This set of $d_v - 1$ independent equations, together with the constraint (51), determines $\nu_{ev}(t)$ for all $e \in E_v$, if the $\nu_{et}$ and $\mu_{et}$ are known. With the aid of (50), (48) reduces to a single equation to determine $\mu_{ev}(t)$:

$$ - \frac{d_v}{2} \mu_{ev}(t) + \sum_{e=1}^{d_v} \int_{-\infty}^{\infty} ds \left( \frac{\partial G_0}{\partial x}(t, 0; s, L_e) \mu_{et}(s) - \sum_{e=1}^{d_v} \int_{-\infty}^{\infty} ds \frac{\partial^2 G_0}{\partial x \partial y}(t, 0; s, L_e) \nu_{et}(s) \right) $$

$$ = - \frac{\partial G_0}{\partial x}(t, 0; s_0, y_0) \sum_{e=1}^{d_v} \delta_{ee_0} . \quad (54) $$

(The last factor in (54) is equal to either 0 or 1, unless $e_0$ is a loop at $v$, in which case it equals 2.)

So as in section 5 we have in (53)–(54) an integral equation of the form

$$ \vec{\mu} = \vec{g}_0 + K \vec{\mu}, \quad (55) $$

where $\vec{\mu}$ is a vector-valued function whose $\sum_v d_v$ components are, for each $v$, any $d_v - 1$ independent choices of the quantities $\nu_{ev}$ (constrained by (51)) and any one of the (equal) quantities $\mu_{ev}$. Of course, in any concrete case the “et” notation needs to be resolved in favor of a fixed labeling of the vertices. In principle all integrals in the Neumann series can be formally evaluated recursively, and the results for $T(t, x; s, y)$ must be the same as those obtained by Wilson [32, 14]. Convergence of the series is not immediately obvious (see Appendix B). However, convergence of the series for the total energy has been proved in [6].

Acknowledgments

This research is supported by National Science Foundation Grant PHY05-54849. Much of the work was done while I enjoyed the hospitality and partial support of the Institute for Mathematics and Its Applications (NSF Grant DMS04-39734) and the Kavli Institute for Theoretical Physics (NSF Grant PHY05-51164). I am grateful for sympathetic audiences and occasional technical help to all my student research assistants (especially Justin Wilson, Zhonghai Liu, and Kevin Resil), the other members of the Texas–Oklahoma–Louisiana vacuum energy research consortium, and the members of the Texas A&M quantum graphs research group (especially Brian Winn for improving the treatment of the integrals in Appendix A).

Appendix A. Evaluation of integrals

Lemma: Let $x$ and $y_0$ be positive. Then

$$ \int_{-\infty}^{\infty} ds \frac{d}{[(t-s)^2 + x^2][(s-s_0)^2 + y_0^2]} = \frac{\pi}{xy_0} \frac{x + y_0}{(t-s_0)^2 + (x+y_0)^2} ; \quad (A.1) $$

$$ \int_{-\infty}^{\infty} (t-s) ds \frac{d}{[(t-s)^2 + x^2][(s-s_0)^2 + y_0^2]} = \frac{\pi}{y_0} \frac{t-s_0}{(t-s_0)^2 + (x+y_0)^2} . \quad (A.2) $$
Proof: Tediously, these integrals can be evaluated by standard methods — either residues or partial fractions. (The point \((t, x) = (s_0, y_0)\) requires special attention with a continuity argument.)

**Proposition:** Let \(x\) and \(y_0\) be positive. Then

\[
\int_{-\infty}^{\infty} ds \ln \left[ \frac{(t-s)^2 + x^2}{(s-s_0)^2 + y_0^2} \right] \frac{1}{s_0 - s} = \frac{\pi}{y_0} \ln \left[ \frac{(t-s_0)^2 + (x+y_0)^2}{(t-s_0)^2 + y_0^2} \right].
\] (A.3)

Proof: Note that differentiating (A.3) with respect to \(x\) yields (A.1), while differentiating (A.3) with respect to \(t\) yields (A.2). It follows that the integral in (A.3) equals the right-hand side of (A.3) plus a constant, \(C\), that is independent of \(x\) and \(t\). The substitution \(\tilde{s} \equiv s - s_0\) reduces the integral to

\[
\int_{-\infty}^{\infty} d\tilde{s} \ln \left[ \frac{(t-s_0 - \tilde{s})^2 + x^2}{\tilde{s}^2 + y_0^2} \right],
\] (A.4)

from which it is easy to see that it is symmetric in \(t\) and \(s_0\). Therefore, \(C\) is independent of \(s_0\) too. To fix \(C\) it suffices to consider the special cases \(x \to 0, t = 0, s_0 = 0\):

\[
C = \int_{-\infty}^{\infty} ds \frac{\ln s^2}{s^2 + y_0^2} - \frac{\pi}{y_0} \ln y_0^2
\]

\[
= \frac{1}{y_0} \int_{-\infty}^{\infty} d\sigma \frac{\ln(\sigma^2 y_0^2)}{\sigma^2 + 1} - \frac{1}{y_0} \ln y_0^2 \int_{-\infty}^{\infty} d\sigma \frac{1}{\sigma^2 + 1}
\]

\[
= \frac{2}{y_0} \int_{-\infty}^{\infty} \frac{\ln \sigma}{\sigma^2 + 1} d\sigma
\]

\[
= \frac{4}{y_0} \left[ \int_{0}^{1} \frac{\ln \sigma}{\sigma^2 + 1} d\sigma + \int_{1}^{\infty} \frac{\ln \sigma}{\sigma^2 + 1} d\sigma \right]
\]

\[
= 0
\]

because the substitution \(\sigma \to 1/\sigma\) converts the second term to the negative of the first.

**Remark:** (A.3) is an instance of a formula given by Balian and Bloch [3, (7.2)],

\[
G_0(\tilde{r}) = 2 \int_S d\sigma_\alpha \frac{\partial G_0(r_\alpha)}{\partial n_\alpha} G_0(\alpha \tilde{r})
\] (A.6)

where \(\tilde{r}\) is the image of \(r\) in the plane \(S\). They conclude it just by noting that in this case the boundary-integral/multiple-reflection expansion must agree with the image solution, assumed previously known. One of the main motivations of the present exercise was to verify (A.6) directly, or, to put it differently, to derive the image solution from the (more general and fundamental) boundary-integral solution. The symmetry of (28) in \((t, x)\) and \((s, y_0)\) is an instance of a symmetry of the right-hand side of (A.6) noted by Hansson and Jaffe [16, (A.12)].

**Appendix B. Convergence issues**

**Appendix B.1. Case 3**

Extrapolating from (43), one can see that the series (41) will not converge, because the terms fall off only linearly with the distance to the image charge. (The corresponding
series for the Dirichlet case is conditionally convergent because of sign alternation.) The series for \( G \), starting with (42) and (44), is even worse: the terms grow logarithmically.

In studying vacuum energy we are usually interested in derivatives of \( T \). Their series converge better, because the differentiations build up powers of \( (t - s)^2 + (y_0 + \cdots)^2 \) in the denominators. One can say that the original series converges distributionally with respect to test functions possessing sufficiently many antiderivatives that are also test functions (in the simplest case, test functions orthogonal to the constant functions).

The standard test for convergence of a Neumann series like (41) is that the norm of \( K \) as an operator from some Banach space into itself be less than 1. In our case (see (36)–(38)) the kernel function is built from

\[
K_0(t, s) = \frac{1}{\pi} \frac{L}{(t - s)^2 + L^2},
\]

so that

\[
\int_{-\infty}^{\infty} ds \ K_0(t, s) = 1 = \int_{-\infty}^{\infty} dt \ K_0(t, s).
\]

It follows that \( K_0 \) has norm 1 as an operator in either \( L^1(\mathbb{R}) \) or \( L^\infty(\mathbb{R}) \). Furthermore, the iterated kernels have the same general form and the same norm; for example,

\[
K_0^2(t, s_0) \equiv \int_{-\infty}^{\infty} ds \ K_0(t, s) K_0(s, s_0) = \frac{1}{\pi} \frac{2L}{(t - s_0)^2 + (2L)^2}
\]

by (A.1). So, in the multiple-reflection expansion we are operating right on the circle of convergence in the plane of a formal parameter multiplying \( K \) ("marginal convergence"). Actually, one apparently needs (B.3) to complete the abstract proof that the operator \( L^1 \)-norm is 1, not possibly something smaller. The foregoing remarks about conditional and derivative convergence show, however, that the latter possibility does not hold here.

Note in passing that \( K_0 \) is certainly not trace class or Hilbert–Schmidt, since \( \int_{-\infty}^{\infty} ds \ K_0^2(s, s) \) is divergent. (The full operator \( K \) of (37) has the matrix-valued kernel

\[
K = \begin{pmatrix} 0 & K_0 \\ K_0 & 0 \end{pmatrix},
\]

which, being totally off-diagonal, has a vanishing trace in the naive sense that

\[
\sum_v \int_{-\infty}^{\infty} ds \ K_{vv}(s, s) = 0,
\]

but that does not make it trace class.) The Fredholm solution is worse than divergent, because even the individual terms in the numerator and denominator series do not exist. Of course, this is to be expected for a convolution integral equation on an infinite interval. (This issue does not arise in the standard literature [11, 2, 3, 22, 30, 31, 8, 28], which concentrates on compact boundaries.) If the graph were to be studied at finite temperature (Appendix C), the interval would be finite and the Fredholm theory would be applicable, possibly providing better convergence than that of the Neumann series.
Appendix B.2. Case 4

The foregoing argument does not readily extend to the integral equation system \((55)\), because the undifferentiated \(G_0\) appearing twice in \((53)\) is not \(L^1\) (nor \(L^\infty\)) in the “time” variables.

At first glance it is not obvious even that the individual terms in the iterative solution will converge. Inspection of \((53)-(54)\), together with \((4)\), \((A.1)\), and \((A.3)\), shows by induction, however, that each term in \(\nu_{ev}(t)\) is logarithmic like \(G_0\) and each term in \(\mu_{ev}(t)\) has behavior like \(\partial G_0/\partial x\) as \(t \to \infty\). (There are always enough spatial derivatives to avert a disaster.) It seems likely that, as in Case 3, one is sitting on the edge of a region of convergence, and the convergence of \(\gamma_e\) can be improved by taking spatial derivatives. (See also the plausibility argument and numerical verification in \([12]\).) However, it is not possible to prove convergence by inspection without control over the number of terms in each order of the series and the magnitudes of their numerical coefficients.

On the question of convergence of the series, some improvement is achieved by changing variables from \(\nu\) to \(\nu'\). Equations \((53)\) and \((54)\) can be rewritten

\[
\begin{align*}
\nu'_{ev}(t) &+ 2 \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial t}(t, 0; s, L_e)\mu_{et}(s) \\
& - 2 \int_{-\infty}^{\infty} ds \frac{\partial^2 G_0}{\partial t \partial y}(t, 0; s, L_e)\nu_{et}(s) + 2 \frac{\partial G_0}{\partial t}(t, 0; s_0, y_0)\delta_{e\epsilon_0} \\
& = \text{same with } e \to f, \tag{B.4}
\end{align*}
\]

\[
\begin{align*}
\mu_{ev}(t) - \frac{2}{d_v} \sum_{\epsilon = 1}^{d_v} \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial x}(t, 0; s, L_e)\mu_{et}(s) + \frac{2}{d_v} \sum_{\epsilon = 1}^{d_v} \int_{-\infty}^{\infty} ds \frac{\partial^2 G_0}{\partial x \partial y}(t, 0; s, L_e)\nu_{et}(s) \\
& = \frac{2}{d_v} \frac{\partial G_0}{\partial x}(t, 0; s_0, y_0) \sum_{\epsilon = 1}^{d_v} \delta_{e\epsilon_0}. \tag{B.5}
\end{align*}
\]

Observe now that

\[
\frac{\partial^2 G_0}{\partial x \partial y}(t, x; y) = \frac{1}{2\pi} \frac{(t-s)^2 - (x-y)^2}{[(t-s)^2 + (x-y)^2]^2} = - \frac{\partial^2 G_0}{\partial s \partial t} \tag{B.6}
\]

and

\[
\frac{\partial G_0}{\partial t}(t, x; y) = - \frac{1}{2\pi} \frac{t-s}{(t-s)^2 + (x-y)^2} = - \frac{\partial G_0}{\partial s}. \tag{B.7}
\]

Some integrations by parts then put the system into the form

\[
\begin{align*}
\nu'_{ev}(t) &+ 2 \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial t}(t, 0; s, L_e)\mu_{et}(s) \\
& - 2 \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial y}(t, 0; s, L_e)\nu'_{et}(s) + 2 \frac{\partial G_0}{\partial t}(t, 0; s_0, y_0)\delta_{e\epsilon_0} \\
& = \text{same with } e \to f, \tag{B.8}
\end{align*}
\]
\[
\mu_{ev}(t) - \frac{2}{d_v} \sum_{e=1}^{d_v} \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial x}(t, 0; s, L_e) \mu_{et}(s) + \frac{2}{d_v} \sum_{e=1}^{d_v} \int_{-\infty}^{\infty} ds \frac{\partial G_0}{\partial t}(t, 0; s, L_e) \nu'_{et}(s) = \frac{2}{d_v} \frac{\partial G_0}{\partial x}(t, 0; s_0, y_0) \sum_{e=1}^{d_v} \delta_{ee_0} \tag{B.9}
\]

Recall that \(e\) and \(f\) are edges attached to the same vertex \(v\), \("t"\) refers to the other vertex of the edge in question, \(e_0\) is the edge containing the source point \(y_0\), and the derivatives are in the direction away from \(v\). Because of constraints (50) and (51), effectively there are \(\sum_v d_v\) independent components of \(\nu'\) and \(\mu\) (twice the number of edges in the graph), although superficially the number of unknowns is twice that, and the number of equations even larger if all pairs \(\{e, f\}\) are counted. Again one can conclude by induction and Appendix A that all terms in the \(\nu'\) and \(\mu\) series are of the same type as their respective source terms in (B.8)–(B.9).

Besides the redundancy of components, there are two technical obstacles to showing that (B.8)–(B.9) manifests an integral operator of norm at most 1. The first is that “time” derivatives of \(G_0\) ([B.7]) do not fall off as fast in the “time” variables as space derivatives ([4]) do. However, one can hope to apply the generalized Young inequality [8, Theorem 0.10] with the weight function \(\rho(s) = (1 + |s|)^{-1}\) in all the integrals. With respect to that measure, every integral kernel in (B.8)–(B.9) is, with respect to the variables \(t\) and \(s\) separately, an \(L^1\) function with norm at most 1 (in view of (B.2) and some trivial estimates). It follows that each term defines a mapping of norm at most 1 in the Banach space \(L^p_{\rho}(1 \leq p \leq \infty)\) of functions such that
\[
\int_{-\infty}^{\infty} |f(s)|^p \rho(s)^{1-p} ds < \infty \tag{B.10}
\]
(if \(p = \infty\), the space of functions such that \(|f(s)|/\rho(s)\) is bounded almost everywhere).

The second obstacle is that each equation contains two such terms, not one, and after redundant components are eliminated from (B.8) via (51) the number of terms will be still larger. Therefore, the obvious bound on the one-sided \(L^1\) norms of the matrix-valued integral kernel is larger than 1, and one cannot conclude by this method that the series even marginally converges.

Appendix C. Finite temperature

The equilibrium state at temperature \(T\) should be described by replacing the usual cylinder kernel by a function periodic in \(t\) with period \(\beta = 1/T\). In general, this construction can be implemented by replacing \(G_0\) by
\[
G_T(t, x; s, y) = \sum_{N=-\infty}^{\infty} G_0(t, x; s - N/T, y) \tag{C.1}
\]
or by solving the partial differential equation with periodic boundary condition directly, or by summing the appropriate eigenfunction expansion with a Boltzmann weighting factor.
In total dimension 2, where $G_0$ is given by (1), the literal (C.1) fails because of divergence. However, by making the arbitrary constants in (1) dependent on $N$ one can arrive at

$$G_T = -\frac{1}{4\pi} \ln[\cosh(2\pi T(x - y)) - \cos(2\pi T(t - s))] + C,$$

(C.2)

whose first derivatives are

$$\frac{\partial G_T}{\partial t} = -\frac{T}{2} \frac{\sin(2\pi T(t - s))}{\cosh(2\pi T(x - y)) - \cos(2\pi T(t - s))},$$

(C.3)

$$\frac{\partial G_T}{\partial x} = -\frac{T}{2} \frac{\sinh(2\pi T(x - y))}{\cosh(2\pi T(x - y)) - \cos(2\pi T(t - s))}.$$  

(C.4)

One can check the correctness of (C.2) by showing that it satisfies all the necessary conditions:

(i) Periodicity in $t$ with minimal period $1/T$.

(ii) Delta-function initial singularity: When $t - s$ and $x - y$ are small, $G_T \approx G_0$, which is known to have the correct behavior.

(iii) Asymptotic behavior at spatial infinity: logarithmic growth, just like $G_0$.

(iv) Partial differential equation

$$\frac{\partial^2 G_T}{\partial t^2} + \frac{\partial^2 G_T}{\partial x^2} = 0.$$  

(C.5)

Moreover, as in (B.6) there holds

$$\frac{\partial^2 G_0}{\partial x \partial y} = -\frac{\partial^2 G_0}{\partial s \partial t}.$$  

(C.6)

Remark: Alternatively, to deduce (C.4) from (C.1), use the identity

$$\sum_{N=-\infty}^{\infty} \frac{1}{a^2 + (b + N)^2} = \frac{\pi}{2a} \{\coth[\pi(a + ib)] + \coth[\pi(a - ib)]\}$$

$$= \frac{\pi}{a} \frac{\sinh(2\pi a)}{\cosh(2\pi a) - \cos(2\pi b)}.$$  

(C.7)

(The first version of this formula was listed in [11]. The simpler final form follows by elementary identities.) Going backward (a Mittag-Leffler expansion), one can get the analogous formula (C.3), and then (C.2) is easy to guess.

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