Investigating the Spectral Geometry of a Soft Wall

J. D. Bouas, S. A. Fulling, F. D. Mera, K. Thapa, C. S. Trendafilova, and J. Wagner

Abstract. The idealized theory of quantum vacuum energy density is a beautiful application of the spectral theory of differential operators with boundary conditions, but its conclusions are physically unacceptable. A more plausible model of a reflecting boundary that stays within linear spectral theory confines the waves by a steeply rising potential function, which can be taken as a power of one coordinate, $z^\alpha$. We report investigations of this model with considerable student involvement. An exact analytical solution with some numerics for $\alpha = 1$ and an asymptotic (semiclassical) analysis of a related problem for $\alpha = 2$ are presented.

1. Introduction

The Casimir effect [9, 8, 29, 27, 6] is an observable attraction between neutral electrical conductors. Its mathematical charm is that, at least for perfect conductors, it can be attributed to and calculated from the geometrical dependence of the energy of the quantized electromagnetic field in the region between the conductors. As often in quantum field theory, naive calculations give an infinite answer. Subtraction of the zero-point energy of each field mode renders the local energy density finite but leaves a nonintegrable singularity at the boundaries. This divergence, because it can be regarded as permanently attached to the conductors, does not interfere with the calculation of the force of attraction between rigid bodies. However, a more accurate representation of the physics near the boundary is needed [3, 20] to understand situations where the boundary can deform, such as the celebrated case of an expandable sphere [7]. Furthermore, the energy density (more completely, the stress tensor) of the field should act as a source of the gravitational field in general relativity, so localized infinities within it are not physically plausible [10]. For more detailed background information see [14, 15, 11, 17, 21].

It is universally agreed among physicists that the root of this problem is that the idealization of a “perfect conductor” is inapplicable to very-high-frequency modes of the quantized field. A full treatment of the physical problem, including modeling of the charged particles inside the conductors, would take us out of the spectral theory
of self-adjoint linear partial differential operators into difficult, nonlinear condensed-matter physics [4]. One might hope that an ad hoc cutoff of the contribution of high-frequency modes would preserve the qualitative essence of the physically correct solution, and indeed a simple exponential cutoff leads to both tractable calculations and physically plausible results [17, 21], while placing the topic firmly within the study of the asymptotics of integral kernels (Green functions) associated with the operator concerned, in the grand tradition of spectral and geometrical asymptotics. (Most of the issues of principle in vacuum energy are adequately addressed by studying a scalar field with Dirichlet boundary conditions instead of an electromagnetic field with perfect-conductor boundary conditions, and our discussion has now lapsed into that setting.)

Unfortunately, a close examination of the stress tensor (in particular, energy density and pressure) predicted by the theory of [17] reveals that the expected energy-balance equation (sometimes called principle of virtual work [5]),

\[
\frac{\partial E}{\partial h} = -\int_{S_h} p,
\]

(1.1)

describing the change in total energy when a boundary acted upon by pressure \( p \) is moved a distance \( h \), is not satisfied [16]. The root of this problem appears to be that the degree to which a particular normal mode is affected by the cutoff depends on \( h \), so that derivatives of the cutoff function contaminate fundamental relations like (1.1). The exponential cutoff on frequency amounts, after analytic continuation, to a time-direction separation of the space-time points that are the argument variables of the integral kernel for the wave equation of the problem. Physically plausible results can be achieved for the various tensor components in various scenarios by choosing a specific space-time direction for the point separation in each case, but such an ad hoc procedure cannot be regarded as logically satisfactory for the long term.

Our present goal is to replace the reflecting boundary and the cutoff with a smooth potential rising to infinity. The potential can be thought of as a static configuration of another scalar field (presumably of very high mass). After some well understood renormalizations in the bulk, this model should yield a finite vacuum stress tensor without any cutoff. As an internally consistent physical system without ad hoc modification, it is expected to satisfy the physically required energy-balance relation. Yet in the limit of a very steep wall it should approach in some sense the vacuum stress of the problem with Dirichlet boundary. If its predictions resemble those for hard-wall calculations with certain point separations, those (technically easier) ad hoc methods will be vindicated and can be used with confidence in other situations.

Here we report progress on this problem achieved during the spring semester of 2010, while J. Wagner held a Visiting Assistant Professorship in Mathematics at Texas A&M University. He worked closely with Professor S. Fulling and four research assistants supported by his NSF grant: mathematics M.S. students J. Bouas and F. Mera and undergraduates (physics-mathematics double majors) C. Trendafilova and K. Thapa. This brief period was notable for intensity of collaboration.
2. The model

Consider the potential function \((1 \leq \alpha \in \mathbb{R}; \mathbf{r} = (x, y, z) \in \mathbb{R}^3)\)

\[
v(\mathbf{r}) = \begin{cases} 
0, & z < 0 \\
\lambda_0 \left(\frac{z}{z_0}\right)^\alpha, & z > 0.
\end{cases}
\]

It is characterized by \(\alpha\) and the single length scale

\[
\hat{z} = \left(\frac{z_0}{\lambda_0}\right)^{\frac{1}{\alpha+2}}.
\]

We ordinarily fix \(\lambda_0 = z_0 = 1\) and let \(\alpha\) vary (and suppress the arguments \(x\) and \(y\)). Thus \(v(1) = 1\) for all \(\alpha\) and the potential forms an increasingly steep wall near \(z = 1\) as \(\alpha \to \infty\) (Fig. 1).

The scalar field is an operator-valued distribution satisfying

\[
\frac{\partial^2 \varphi}{\partial (x^0)^2} = \nabla^2 \varphi - v(z)\varphi.
\]

Because the PDE \((2.2)\) is linear and invariant under translation in time \((x^0)\), it has a standard reduction to a classical eigenvalue problem: \(\varphi(x^0, x, y, z)\) is a linear superposition (an integral, since the spectrum in our model will be continuous) of normal modes of the form \(\phi_j(\mathbf{r})e^{\pm i\omega_j x^0}\) with operator coefficients. For the details we refer to \([29, 17]\). The physical quantities of interest are (the vacuum expectation values of) the components of the energy-momentum tensor, especially the energy density

\[
T^{00}(\mathbf{r}) = \frac{1}{2} \left\{ \left(\frac{\partial \varphi}{\partial x_0}\right)^2 - \varphi \nabla^2 \varphi + v\varphi^2 \right\}.
\]

These expectation values can be expressed as derivatives of the cylinder kernel (Poisson kernel) of the differential operator on the right-hand side of \((2.2)\), which can be defined by the PDE

\[
\left(\frac{\partial^2}{\partial t^2} + \nabla^2 - v(z)\right) \widetilde{T}(t, x, y, z, z') = 2\delta(t)\delta(x)\delta(y)\delta(z - z')
\]

or by the eigenfunction expansion

\[
\widetilde{T}(t, \mathbf{r}, \mathbf{r}') = -\int d\mu(j) \omega_j^{-1} \phi_j(\mathbf{r})\phi_j(\mathbf{r}') e^{-\omega_j t},
\]

\(^1\)We take \(\hbar = 1 = c\), curvature coupling constant \(\xi = \frac{1}{4}\), and metric signature \(g_{00} < 0\).
where \( \mu \) is a properly normalized spectral measure over the index set. \( T \) is an analytic continuation via \( t = i(x - x') \) of the Green function of the wave equation \((2.2)\). In \((2.5)\) we take advantage of the translational invariances of \((2.2)\) to set \( x' = y' = 0 \) without loss of generality. Now (formally)

\[
T^{00} = -\frac{1}{2} \left. \frac{\partial^2 T}{\partial t^2} \right|_{t=0,x=0=y,z=z},
\]
and there are similar formulas (involving derivatives with respect to the spatial variables) for the three pressures, \( P_z = T^{zz} \) etc. As usual, we must refer to the references for complete explanations.

In \((2.6)\) and similar formulas, the integral kernel is being evaluated at equal arguments ("on diagonal" or "in the coincidence limit", depending on whether one is in mathematics or physics literature). In studying a new model it is common to look first at the diagonal value of \( T \) itself (without any derivatives), which has the physical interpretation of vacuum expectation value of the square of the field \( \phi \).

### 3. Analytical solution

#### 3.1. Eigenfunctions

Solving \((2.2)\) by separation of variables is a standard exercise in quantum scattering theory. The formal index \( j \) in \((2.5)\) is a triple \( (k_x, k_y, p) \) with \( k_\perp \equiv (k_x, k_y) \in \mathbb{R}^2 \) and \( p \in (0, \infty) \). The frequency \( \omega_j \) is the positive solution of

\[
\omega^2 = k_\perp^2 + p^2.
\]

The eigenfunction is

\[
\phi_j(r) = (2\pi)^{-1} e^{i k_\perp \cdot r} \phi_p(z)
\]

where

\[
\left( -\frac{\partial^2}{\partial z^2} + v(z) - p^2 \right) \phi_p(z) = 0.
\]

When \( z < 0 \), it must take the form

\[
\phi_p(z) = \sqrt{\frac{2}{\pi}} \sin[pz - \delta(p)]
\]

for some real phase shift \( \delta(p) \) (not to be confused with the Dirac \( \delta \) in \((2.4)\) and \((3.24)\)). The normalization factors in \((3.1)\) and \((3.3)\) guarantee that the spectral measure \( \mu \) is 3-dimensional Lebesgue measure.

When \( z > 0 \), \( \phi \) is best expressed as

\[
\phi_p(z) = C(p) P_\alpha(z/z_0, (\hat{z}p)^2)
\]

where the function \( P_\alpha(z, E) \) is a solution of

\[
\left( -\frac{d^2}{dz^2} + z^\alpha - E \right) P_\alpha(z, E) = 0
\]

that vanishes as \( z \to \infty \). For small, integer \( \alpha \) the solutions are known as Airy functions and parabolic cylinder functions:

\[
P_1(z, E) \propto Ai(z - E), \quad P_2(z, E) \propto D_{\frac{1}{2}(E-1)}(\sqrt{2}z).
\]

For a hard wall at \( z_0 \), we have \( P_\infty(z, E) \propto \sin[\sqrt{E}(z - z_0)] \). Henceforth we take \( \hat{z} = z_0 = 1 \) so that \( E = p^2 \).
The solutions and their derivatives must match at \( z = 0 \). Thereby \( C \) and, more importantly, \( \delta \) are determined:

\[
\tan(\delta(p)) = -p \frac{P_\alpha(0, p^2)}{P'_\alpha(0, p^2)},
\]

\[
C(p)^2 = \frac{2}{\pi} \frac{1}{P_\alpha(0, p^2)^2 + p^{-2}P'_\alpha(0, p^2)^2}.
\]

Even in the cases (3.6) these formulas do not lend themselves to exact evaluation of the integrals for energy density and pressure, so further approximation or qualitative analysis is needed.

### 3.2. Asymptotics.

When \( p = 0 \) the solution of (3.5) is known (a modified Bessel function):

\[
P_\alpha(z, 0) = z^{1/2} K_{\frac{\alpha}{2}} \left( \frac{2}{\alpha + 2} z^{\frac{\alpha + 2}{2}} \right).
\]

For small \( p \) the solution can therefore be constructed as a perturbation expansion:

\[
P_\alpha(z, E) = P_\alpha(z, 0) + EP_\alpha^{(1)}(z) + \cdots.
\]

This process requires constructing the Green function (resolvent kernel) for the nonhomogeneous unperturbed equation and applying it iteratively. In this way we find that

\[
\delta(p) = p(\alpha + 2) \frac{2}{\alpha + 2} \Gamma \left( \frac{\alpha + 3}{2} \right) \Gamma \left( \frac{\alpha + 1}{2} \right) + O(p^3).
\]

Fortunately, the Bessel-function integral needed to find the \( O(p^3) \) term can be evaluated in closed form, but we do not report the result here.

At large \( p \) one can construct a WKB (semiclassical) approximation:

\[
\phi_p(z) \sim [p^2 - v(z)]^{-\frac{1}{4}} \cos \left[ \int_{z}^{a} \sqrt{p^2 - v(\tilde{z})} \, d\tilde{z} - \frac{\pi}{4} \right],
\]

where \( a = p^{2/\alpha} \) is the turning point. It follows that

\[
\delta(p) \sim \int_{0}^{a} \sqrt{p^2 - v(z)} \, dz + \frac{\pi}{4} \text{ mod } \pi.
\]

Closer examination shows that the "mod \( \pi \)" can be ignored and the integral evaluated as a beta function:

\[
\delta(p) = \frac{1}{\alpha} p^{1+2/\alpha} B \left( \frac{3}{2}, \frac{1}{\alpha} \right) + \frac{\pi}{4} + o(1).
\]

In summary, we have for \( \alpha = 1 \) (the Airy function)

\[
\delta(p) \sim \begin{cases} 
\frac{3^{2/3} \Gamma(\frac{3}{4}) / \Gamma(\frac{1}{4})}{2 \pi^{1/2}} \frac{1}{\alpha}, & p \to 0, \\
\frac{3^{2/3} \Gamma(\frac{3}{4}) / \Gamma(\frac{1}{4})}{2 \pi^{1/2}} \frac{1}{\alpha}, & p \to \infty,
\end{cases}
\]

and for \( \alpha = 2 \) (the parabolic cylinder function)

\[
\delta(p) \sim \begin{cases} 
\frac{2p \Gamma(\frac{3}{4}) / \Gamma(\frac{1}{4})}{2 \pi p^{1/2}} \frac{1}{\alpha}, & p \to 0, \\
\frac{2p \Gamma(\frac{3}{4}) / \Gamma(\frac{1}{4})}{2 \pi p^{1/2}} \frac{1}{\alpha}, & p \to \infty.
\end{cases}
\]

We are interested in the power potential (2.1) only as a convenient model with suitable qualitative properties. Since the function \( \delta(p) \) completely encodes the
influence of the potential on the field in the potential-free region, it is tempting to forget the potential and study the class of models parametrized by functions $\delta$ in a suitable class. The asymptotic relations (3.11) and (3.13) give some idea of what an allowed $\delta$ must look like, but otherwise the inverse problem of determining $\nu$, or even its basic qualitative properties, from a given $\delta$ is wide open, as far as we know. Later we shall show evidence that slight changes in $\delta$ can produce unacceptable results.

### 3.3. The renormalized cylinder kernel.

To exploit the symmetry between $t$ and $r_\perp$ in this problem, we introduce another layer of Fourier transformation into (2.5):

$$T(t, r_\perp, z, z') = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} d\omega \, dk_\perp \int_0^\infty dp \, e^{i\omega t} e^{ik_\perp \cdot r_\perp} \phi_p(z) \hat{T}(\omega, k_\perp, p),$$

where $\omega$ has now become an independent parameter.

The integral over $\mathbb{R}^3$ can be done by standard methods, resulting in

$$\hat{T}(\omega, k_\perp, p) = -\frac{2}{(2\pi)^{3/2}} \frac{\phi_p(z')}{\omega^2 + k_\perp^2 + p^2},$$

where $\omega$ has now become an independent parameter.

The integral over $\mathbb{R}^3$ can be done by standard methods, resulting in

$$T(t, r_\perp, z, z') = -\frac{1}{2\pi} \int_0^\infty dp \, Y(s, p) \phi_p(z) \phi_p(z'),$$

$$Y(s, p) \equiv e^{-sp/s}, \quad s \equiv \sqrt{t^2 + |r_\perp|^2}.$$

We shall concentrate for now on the potential-free region, $z < 0$, where

$$T = -\frac{1}{\pi^2} \int_0^\infty dp \, Y(s, p) \sin(pz - \delta(p)) \sin(pz' - \delta(p)).$$

Upon converting the product of sines to a sum of cosines in the standard way, one sees that the first term is just the “free” kernel that would apply in $\mathbb{R}^4$ if the potential were not there:

$$T = -\frac{1}{2\pi^2} \frac{1}{t^2 + r_\perp^2 + (z - z')^2} + \frac{1}{2\pi^2} \int_0^\infty dp \, Y(s, p) \cos(p(z + z') - 2\delta(p))$$

$$= T_{\text{free}} + T_{\text{ren}}.$$

For a hard (Dirichlet) wall at $z = z_0$ we have $\delta(p) = z_0p$ and hence the well known image solution,

$$T_{\text{ren}} = \frac{1}{2\pi^2} \frac{1}{t^2 + r_\perp^2 + (z + z' - 2z_0)^2}.$$

Before continuing it is instructive to take a close look at this case. $T_{\text{free}}$ is, of course, singular on the diagonal ($t = 0$, $r_\perp = 0$, $z' = z$) and only there. The singularity makes it impossible to pass to the diagonal directly in (2.6), but that is also unnecessary: $T_{\text{free}}$ is present in all problems, including empty space (where $T^{\mu\nu}$ is naturally defined to be zero), and hence is physically meaningless. One expects to isolate and discard it before implementing (2.6), which is applied only
to the “renormalized” kernel, $T_{\text{ren}}$. The latter, as given in (3.21), is nonsingular in the region of physical interest; on diagonal one gets (with our convention $z_0 = 1$)

$$T_{\text{ren}} = \frac{1}{8\pi^2} \frac{1}{(z - 1)^2}$$

and similar formulas (proportional to $(z - 1)^{-4}$) for the energy density and pressures. In the present case (3.19) is applicable over the whole range $-\infty < z < 1$, and (3.22) gives the expectation value of the scalar field right up to the wall (where it develops a nonintegrable divergence). This much is totally standard and familiar to all workers in the field of vacuum energy. However, let us go back to the integral form of (3.21) contained in (3.20):

$$T_{\text{ren}} = \frac{1}{2\pi^2} \int_0^\infty dp \, \frac{e^{-sp}}{s} \cos\left(p(z + z') - 2p\right),$$

where $s = \sqrt{t^2 + |r_\perp|^2}$, and attempt to set $t$ and $r$ equal to 0 before evaluating the integral. Although $T_{\text{ren}}$ is well-defined except when $z + z' = 2$, in (3.23) we appear to have a double disaster: the denominator of the integrand is identically zero, and, moreover, even the integral of the numerator alone diverges because the exponential cutoff is lost. The resolution of this apparent paradox is that

$$\int_0^\infty \cos pz \, dp = \pi \delta(z)$$

in the sense of distributions, and the Dirac distribution $\delta(z)$ is identically 0 for $z \neq 0$. Thus the classically divergent numerator integral is equal to 0 in the distributional sense in the limit $s \to 0$, and (3.23) is consistent with (3.21) and (3.22) there.

Returning to the general case, we are confronted by the integral

$$T_{\text{ren}} = \frac{1}{2\pi^2} \int_0^\infty dp \, \frac{e^{-sp}}{s} \cos\left(p(z + z') - 2\pi^2\right).$$

One might consider evaluating it numerically, given a trustworthy formula or ansatz for $\delta(p)$. However, in view of the previous special example, it is not surprising that the integral is poorly convergent when $s \equiv \sqrt{t^2 + |r_\perp|^2}$ is small, which is precisely where we want it. In fact, we should be able to take $s = 0$ and get a finite answer when $z + z' > 0$, but instead we have the same apparent infinities as in the Dirichlet case; and this time it is not obvious that the integral (without the factor $(z - 1)^{-4}$) vanishes distributionally to lowest order in $s$ when $z + z' > 0$, although that must surely be true.

To compound the problem, it appears that even this weak kind of convergence depends sensitively on $\delta$. Suppose that instead of (3.23) we had considered

$$\frac{1}{2\pi^2} \int_0^\infty dp \, \frac{e^{-sp}}{s} \cos\left(p(z + z') - 2p + \frac{\pi}{2}\right),$$

which one might naively think to correspond to the large-$\alpha$ limit of (3.13) (which actually is invalid for $\alpha \to \infty$ with fixed $p$). This integral equals

$$\frac{1}{2\pi^2} \frac{z + z' - 2}{\sqrt{t^2 + |r_\perp|^2}^2} \frac{1}{t^2 + \|r_\perp\|^2 + (z + z' - 2)^2}.$$

Thus the cancellation that removes the divergence on the $z$ axis in (3.23) does not happen here. More generally, there is a genuine divergence for $\delta(p) = Ap + B$ unless $B = 0$. Naively one would think that the divergent boundary energy we are
studying is contributed by the modes of large $p$, and that therefore only the leading
term in the WKB asymptotics (3.13) would be significant; the current example
shows that that is not true. The fallacy in the reasoning is that high frequency can
correspond to large $k_\perp$ at fixed $p$, as well as to large $p$.

The sensitivity of (3.23) to a constant phase shift remains visible in the polar
framework treated in the next subsection. The $u$ integral in (3.27) or (3.28) in that
case evaluates to a Bessel function $J_1$, which decays slowly as $\rho \to \infty$; however,
the outer integration yields (3.22) by a standard formula found in handbooks and
known to Mathematica. But the tiniest phase shift augments the Bessel function
by a Struve function, which approaches a nonzero constant at infinity, so that the
integral diverges unambiguously.

3.4. Polar coordinates. Therefore, we recast the integration so that all high
frequencies are treated on an equal footing. Any true divergence must come from the
integral over high frequencies, since the eigenfunctions are smooth and bounded.

Abandoning the key formula (3.25) for now, we return to (3.16), which in the
notations $Z \equiv z + z'$, $s = (t, r_\perp)$, $v = (\omega, k_\perp)$, becomes

\[
T_{\text{ren}} = \frac{1}{4\pi^2} \int_0^\infty dp \int_{\mathbb{R}^3} dv \frac{e^{iv \cdot s}}{v^2 + p^2} \cos(pZ - 2\delta(p)).
\]

(Note that $s \equiv |s|$ is the same $s$ as before.) Now introduce polar coordinates in
the space of variables $(p, v_1, v_2, v_3)$, with the main axis in the $Z$ direction and the
prime meridian through $s$ (that is, $s_2 = 0 = s_3$). After several steps of calculation
one arrives at the new key formula

\[
T_{\text{ren}} = \frac{1}{\pi^3} \int_0^\infty d\rho \int_0^1 du \rho^{-1} \sin(s\rho \sqrt{1 - u^2}) \cos(Z\rho u - 2\delta(\rho u)).
\]

Because of the sine, the integrand is not singular, although it needs to be defined
by a limit when $s = 0$. Ultimately we would like to take derivatives of (3.28) and
then pass to the diagonal, but for now we set $s = 0$ and $z = z'$ immediately:

\[
T_{\text{ren}}(0, 0, 0, z, z) = \frac{1}{\pi^3} \int_0^\infty d\rho \int_0^1 du \rho^2 \sqrt{1 - u^2} \cos(2z\rho u - 2\delta(\rho u)).
\]

(As previously remarked, this should yield the expectation value of $\varphi^2$ at $z$.)

The change of variables has not eliminated the problem, but it has isolated it
at the upper limit of a single improper integral. The convergence of (3.28) is
still delicate. Numerical and analytical investigations of it are ongoing. Were it
not for the convergence issues, one could prove easily from (3.28) that the function
manifests approximately inverse-square decay resembling (3.22), but with the
effective wall position $z = 1$ replaced by $z = c$, where $c$ is the coefficient of the
linear term in (3.11). Numerical integrations have been performed in Mathematica
for $\alpha = 1$. Despite the instability of the highly oscillatory integrals, the results are
qualitatively as expected, approaching $(z - c)^{-2}/8\pi^2$ already for moderately large
$|z|$ (Fig. 2).

As this paper was being drafted, K. Milton et al. reported (privately; cf. [28])
an independent evaluation of $T_{\text{ren}}$ for $\alpha = 1$ using a different integral representation
with better convergence properties. They find a weak $(z^{-1})$ divergence in the energy
density at the origin, which in hindsight is to be expected as diffraction from the
coefficient singularity there (which will become less important for larger $\alpha$). The
corresponding singularity in $\bar{T}$ is of order $z \ln |z|$, therefore not visible in Fig. 2.
3.5. Conclusions. Our principal results are the Cartesian formula (3.25), the polar formula (3.27), and the latter’s diagonal specialization (3.28), along with the formula (3.7) for $\delta$ and the asymptotic analyses in the subsection following it. Formulas for energy density and pressure can be obtained by differentiating (3.27) and again passing to the diagonal. Granted the convergence of the integrals, it can be seen that $T_{00}$ and $T_{11}$ (the pressure in the $x$ direction) are equal and opposite, so that (1.1) is satisfied in the sideways motion of a plane partition perpendicular to the plane wall. This happy result, which fulfills the main motivation of the project, follows from the finiteness of the diagonal values (in the potential-free region) of the kernel $T_{\text{ren}}$ and its derivatives without the need of an artificial cutoff, since it is satisfied by the individual normal modes in the integrand.

3.6. Inside the wall. Detailed calculations in the region $z > 0$ have not yet been attempted, since we want to exploit fully the more elementary calculations in $z < 0$ first. Also, one may reasonably consider the energy and stress in that region to be part of the wall, not part of the cavity containing the field. Nevertheless, in our setup the properly renormalized stress tensor inside the wall should still be finite and display the physically sensible behavior (1.1). (Most of the arguments of the previous subsection still apply here, or can be adapted.)

On general grounds one knows that the renormalization will require subtraction of additional terms from $T$. In a nonsingular model the diagonal divergences in $T$ and hence $T^{\mu\nu}$ are determined [13] by the well known small-time divergences of the heat (or quantum) kernel [18, 32]. Wherever the potential $v(r)$ is not zero, the energy density calculated with the standard ultraviolet cutoff ($t$ held nonzero) has the expansion

$$\pi^2 T^{00} \sim \frac{3}{2} t^{-4} - \frac{1}{8} vt^{-2} + \frac{1}{32} (v^2 - \frac{1}{3} \nabla^2 v) \ln t \quad \text{as } t \to 0. \tag{3.29}$$

The first term corresponds to the universal vacuum energy that has been removed by subtracting the free kernel at (3.20). The other terms in (3.29) can be removed by subtracting higher-order terms in the small-$t$ expansion of the exact $T$ (obeying (2.3) with the potential included). Physically, such terms represent redefinitions of the constants in the equation of motion of the $v$ field itself.
A technical issue that must ultimately be addressed here is the validity of (3.20) when \( v \notin C^\infty \). In particular, for \( \alpha = 1 \) (3.29) predicts a Dirac delta at \( z = 0 \) from the term \( \nabla^2 v \), and we will not trust the numerical coefficient until a direct calculation has been carried out. The issue here is the same one that arises in the heat kernel (and Gauss–Bonnet theorem) for the Laplacian in a region in the plane: The contributions of the corners of a polygon cannot be obtained by naively taking the limit of the effects of the curvature of a smooth boundary. This is an interesting question to be investigated in the future.

4. Semiclassical analysis

4.1. General remarks. Separation of variables, even when it is available, is not always the best way to obtain information about the integral kernels (and spectral measures) associated with a linear partial differential operator. Leading terms such as those in (3.29) are routinely found by direct construction of some kernel as an asymptotic series. Higher-order information can be obtained from terms in the quantum kernel (Green function of the time-dependent Schrödinger equation) corresponding to periodic orbits of the underlying classical mechanical system \([1, 2, 19, 34]\). (These terms are also present in the heat kernel but exponentially suppressed. They produce oscillatory terms in the averaged eigenvalue density.)

The construction of Green functions for the Laplace and Helmholtz equations in bounded domains in \( \mathbb{R}^n \) (billiards) by reduction to integral equations on the boundary is well known. The counterpart construction for the heat equation is less familiar but available in the literature \([22, 30]\). What is seldom appreciated is that for the heat equation the solution of the boundary integral equation by iteration is convergent, because the integral operator has Volterra structure. One therefore has, in principle, an explicit construction of the solution. The Schrödinger equation has the same Volterra structure, so one expects again to have a convergent series solution. To implement this idea in a general context, Mera \([25]\) has proved the following general Volterra theorem:

**Theorem 4.1.** Let the kernel \( A(t, \tau) \) be (for each \( t \) and \( \tau \) in an interval \( I \)) a uniformly bounded linear operator \( A: \mathcal{B} \to \mathcal{B} \), where \( \mathcal{B} \) is a Banach space, and suppose that it has the Volterra property, \( A(t, \tau) = 0 \) when \( \tau > t \). Define the integral operator \( Q: L^\infty(I; \mathcal{B}) \to L^\infty(I; \mathcal{B}) \) by

\[
Q\phi(t) = \int_0^t A(t, \tau)\phi(\tau) \, d\tau.
\]

Then the Volterra integral equation

\[
\phi - Q\phi = f \quad (f \in L^\infty(I; \mathcal{B}))
\]

can be solved by successive approximations. That is, the Neumann series converges in the topology of \( L^\infty(I; \mathcal{B}) \).

The application of the theorem in any particular context reduces to showing that the operator family \( A(t, \tau) \) is uniformly bounded on a suitable space \( \mathcal{B} \). For Schrödinger equations this is a nontrivial task and requires supplementary technical assumptions. Here we are primarily interested in problems with potentials in \( \mathbb{R}^n \). In that setting the key idea, due to Balian and Bloch \([2]\), is to let the semiclassical or WKB approximation to the quantum kernel play the role played by the free kernel in
billiard problems, so that the role played by scattering off the boundary in billiards (or by scattering by the potential in standard time-dependent perturbation theory [24, Ch. 7][25]) is played here by scattering by a source that is essentially the residual error in the WKB approximation to the exact kernel. This construction is developed in [24, Ch. 8].

The WKB kernel is

\[ G_{\text{scl}}(x, t; y, 0) = (2\pi \imath \hbar)^{-n/2} A e^{iS/\hbar}, \]

where

\[ S(x, y, t) = \int_0^t L(q(\tau), \dot{q}(\tau)) d\tau, \quad L = \frac{1}{2} \dot{q}^2 - v(q), \]

is the classical action, a solution of the Hamilton–Jacobi equation, and the amplitude \( A \) is

\[ A(x, y, t) = \sqrt{\det \left( -\frac{\partial^2 S}{\partial x_i \partial x_j} \right)} . \]

If there is more than one classical trajectory \( q(\tau) \) starting at \( y \) at time 0 and arriving at \( x \) at time \( t \), the semiclassical approximation is a sum of such terms, possibly modified by Maslov phase factors (see next subsection) to keep track of places where the radicand in (4.5) has gone negative.

Define a kernel \( Q \) by

\[ Q(x, t; y, \tau) = \hbar^2 \left| \Delta x A(x, t; y, \tau) \right| e^{iS(x, t; y, \tau)} . \]

The corresponding operators \( Q \) and \( G_{\text{scl}} \) are related by

\[ (-i\hbar \partial_t - \hbar^2 \nabla^2 + v(x)) G_{\text{scl}} = 1 - Q ; \]

that is, \( Q = O(\hbar^2) \) is the amount by which \( G_{\text{scl}} \) fails to solve the PDE for which it was devised. Thus, formally,

\[ G = G_{\text{scl}} \sum_{j=0}^{\infty} Q^j , \]

or

\[ G(x, t; y, \tau) = G_{\text{scl}}(x, t; y, \tau) + \int_0^t \Gamma(t, \tau_1) \Lambda(\tau_1, \tau) d\tau_1 + \cdots , \]

where

\[ [\Gamma(t, \tau) \phi(\tau)](x) = \int_{\mathbb{R}^n} G_{\text{scl}}(x, t; y, \tau) \phi(y, \tau) dy , \]

\[ [\Lambda(t, \tau) \phi(\tau)](x) = \int_{\mathbb{R}^n} Q(x, t; y, \tau) \phi(y, \tau) dy . \]

**Theorem 4.2.** [24] In the notation of the two foregoing paragraphs: Suppose that the following two hypotheses hold:

1. \( \left\| \frac{\Delta A}{A} \right\|_{L^\infty(I^2, \mathbb{R}^{2n})} < \infty . \)
2. \( \Gamma \) is a bounded operator from \( L^2(\mathbb{R}^n) \) to itself.

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2In this section \( x \) and \( y \) are two different spatial points, not coordinates of the same point as earlier, and we reintroduce \( \hbar \) to make the structure of the semiclassical asymptotics clearer. To simplify the Schrödinger equation we take the mass \( m = \frac{1}{2} \).
Then the semiclassical operator $\Lambda: L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is a bounded linear integral operator. It follows that the Volterra integral equation in the space $L_{\infty}^{-2}(I; \mathbb{R}^n)$ with the semiclassical kernel $Q(x, t; y, \tau)$ can be solved by successive approximations.

This construction implements the Feynman path integral idea in a way different from the usual time-slicing approach. Each term in (4.9) is an integral over classical paths with $j$ scatterings off an effective potential $\Delta A/A$.

The determinant in (4.5) is singular at caustics, where the mapping from initial velocity data (at $y$) to $x$ ceases to be a diffeomorphism. One can expect both conditions (1) and (2) to be problematical if the orbit goes through a caustic, but we provide some evidence below that the situation is not as bad as one might expect. A way to go beyond caustics (if necessary) is provided by the Maslov theory [23], as already implemented in a similar problem in [33].

4.2. The harmonic oscillator and the quadratic wall. It was natural to apply Theorem 4.2 to a power potential, with two motivations: to test the validity of the two hypotheses in the theorem in the context of a concrete problem, and to seek new information about the spectral density (and hence eventually the vacuum energy) for a soft wall. We have studied the case $\alpha = 2$ in one dimension,

$$(4.12) \quad v(x) = \begin{cases} 0 & \text{if } x \leq 0, \\ \frac{1}{4} \omega^2 x^2 & \text{if } x > 0. \end{cases}$$

The two transverse dimensions can be ignored because their contribution to the quantum kernel in dimension 3 is a trivial factor.

Consider points $x$ and $y$ that are both in the potential-free region, and a time $t > 0$. There is always a force-free motion directly from $y$ to $x$ in time $t$. It is elementary to calculate for this direct path

$$(4.13) \quad S = \frac{(x - y)^2}{4t}, \quad A^2 = \frac{1}{2t}, \quad \Delta A = 0,$$

so that (of course) the quantum kernel (4.3) is just that of a free particle.

If $\omega t > \pi$ there is another classical path that enters the harmonic-oscillator region at

$$(4.14) \quad \tau = t_1 = \frac{y}{x + y} \left( t - \frac{\pi}{\omega} \right),$$

and reemerges after half a period, at $t_2 = t_1 + \pi/\omega$. This path also contributes to the leading term, $G_{\text{scl}}$, in (4.9). (Bear in mind that such contributions are always of the schematic form $Ae^{iS}$, which we shall not constantly repeat.) We shall see
that the action of the portion of the orbit inside the potential is 0, so the total action is just that of the two free motions at the ends:

\[
S = \frac{y^2}{4t_1} + \frac{x^2}{4(t-t_2)} = \frac{(x+y)^2}{4 \left(t - \frac{\pi}{\omega}\right)}, \quad A^2 = -\frac{1}{2 \left(t - \frac{\pi}{\omega}\right)}, \quad \Delta A = 0.
\]

Note that the resulting term added to \(G_{scl}\) differs by a time translation (and a phase, since \(A^2\) is negative) from the image term that would be produced by a hard wall. We shall show that the proper phase factor is \(-i\). There is an apparent singularity in (4.15) at \(\omega t = \pi\) that deserves closer examination.

Theorem 4.2 is formulated in [24] for a \(C^\infty\) potential. For (2.1), in addition to (4.15) there are waves diffracted from the coefficient singularity at \(z = 0\), but they become increasingly negligible with increasing \(\alpha\).

Now consider \(x\) and \(y\) both inside the potential. From (4.4) and the relevant solution of the classical equation of motion one can reproduce well known formulas,

\[
S(x, y, t) = \frac{\omega}{4\sin(\omega t)} \left[(x^2 + y^2) \cos(\omega t) - 2xy\right],
\]

\[
A^2 = \frac{\omega}{2\sin(\omega t)}, \quad \Delta A = 0.
\]

We need these formulas only for \(0 < \omega t < \pi\); however, for the full harmonic oscillator potential on the whole real line it is well known [23, 31] that the resulting (Mehler) formula for \(G_{scl}\) remains valid everywhere in space-time and gives the exact quantum kernel, with the caveat that (as suggested by the sign change in (4.17)) the kernel must be multiplied by \((-i)^\mu\) where \(\mu\) is the number of occasions when \(t\) has passed through an integer multiple of \(\pi/\omega\). (Conventionally one redefines \(A^2\) and \(A\) to be always positive numbers and writes the Maslov phase factor \((-i)^\mu\) separately.)

At such a time there is a caustic: all the trajectories from \(y\) refocus at \(x = (-1)^\mu y\), \(t = \pi/\omega\). But the kernel formula (4.3) reproduces there the original \((t = 0)\) singularity, which is still a solution of the homogeneous Schrödinger equation. (This situation is strikingly different from that for elliptic equations, such as the time-independent Schrödinger equation, where a caustic marks the breakdown of the semiclassical approximation. Note that the celebrated turning points of the harmonic oscillator are not caustics for the time-dependent problem!)

With this background understanding we can finish treating the trajectory (4.15):

- A variant of the calculation leading to (4.16) shows that, as claimed, \(S = 0\) for any trajectory linking \(y = 0\) to \(x = 0\) (necessarily in elapsed time \(\pi/\omega\)).
- As for the harmonic-oscillator kernel, the singularity in \(A\) of (4.15) is harmless; the companion factor \(e^{S/\hbar}\) is effectively 0 there.
- By continuity from the (purely harmonic) case \(y = 0\), when \(y < 0\) but small one would expect a caustic to occur somewhere near \(x = -y, t = \pi/\omega\). Therefore, when the trajectory reemerges from the potential, this term of the kernel should be multiplied by a Maslov factor \(-i\).

To verify this last claim, and to make a start on computing the second (single-reflection) term in (4.9), we consider a path that starts at \(y < 0\) at time 0 and ends at \(x > 0\) at time \(t\). It must cross the time axis at a time \(t_1\), and from the solution of the classical equation one finds

\[
\omega xt_1 + y \sin(\omega(t - t_1)) = 0,
\]
which can’t be solved by elementary functions. The action is
\[(4.19) \quad S(x, y, t) = \frac{y^2}{4t_1} + \frac{y^2}{8\omega t_1^2} \sin(2\omega(t - t_1)).\]

By implicit differentiation of (4.18) one can find that
\[(4.20) \quad A^2 = \frac{y}{2t_1} \frac{1}{x - y \cos(\omega(t - t_1))}.\]

There will be a caustic if the denominator of (4.20) changes sign. (Since that factor arises from $\partial t_1/\partial x$, its vanishing says that $t_1$ (hence $y$) can vary without changing $x$ (at least to first order).)

To investigate further it is helpful to introduce dimensionless variables
\[(4.21) \quad T = \omega t, \quad \Omega = \omega t_1, \quad 0 < \tilde{\Omega} = T - \Omega < \pi, \quad \rho = -\frac{y}{x} > 0.\]

Then (4.18) is
\[(4.22) \quad 0 = \rho \sin(\tilde{\Omega}) + \tilde{\Omega} - T \equiv f(\tilde{\Omega}) \quad (0 < \tilde{\Omega} < \pi),\]

which can be investigated graphically as the intersection of a trigonometric graph and a straight line. The number of intersections can be 0, 2, or 1 (Fig 4). There is one solution if $T < \pi$ (that is, the straight line hits the axis below the sine curve). There are no solutions if $\rho \leq 1$ and $T > \pi$, or if $\rho > 1$ and $T > T_*$, where
\[(4.23) \quad T_* = \sqrt{\rho^2 - 1} + \cos^{-1} \left( -\frac{1}{\rho} \right).\]

There are two solutions if $\rho > 1$ and $\pi \leq T < T_*$. Finally, there is one solution if the straight line is tangent to the sine curve — that is, $f'(\tilde{\Omega})$ and $f(\tilde{\Omega})$ are zero simultaneously — which happens when $\rho \geq 1$ and $T = T_*$. Furthermore,
\[(4.24) \quad 0 = f'(\tilde{\Omega}) = \rho \cos(\tilde{\Omega}) + 1\]
is the condition for the vanishing of the denominator of (4.20).

Now consider a fixed trajectory with a moving endpoint (that is, fix $y$ and $t_1$ and let $x$ and $t$ vary). When $t \approx t_1$, $f'(\tilde{\Omega})$ is large and positive ($\rho \to +\infty$, $\cos(\tilde{\Omega}) \to 1$). Near the exit point, $t \approx t_2$, $f'(\tilde{\Omega})$ is large and negative ($\rho \to +\infty$, $\cos(\tilde{\Omega}) \to -1$). Therefore, every trajectory does pass through a solution of (4.24) somewhere on its retreat from the potential.

In future work we hope to complete the calculation of $\Delta A$ for trajectories with an endpoint inside the potential. That will enable one to study whether the two
conditions in Theorem 4.2 are satisfied in spite of the caustic, as they are for the Mehler kernel. If so, then one can tackle the second (single-reflection) term in (4.9) by concatenating a trajectory of the sort just studied with one of the time-reversed type. For given \((x, y, t)\) outside the potential, one must integrate over all \((q, \tau)\) inside the potential for which such a trajectory exists. From the taxonomy of paths given above, it is clear that as many as four trajectories can exist, so the term \(G_{\text{sc}}Q^1 = \int \Gamma \Lambda\) is a sum of four terms, each with a domain of integration that is a nontrivial subset of the region \(0 < q < \infty, 0 < \tau < t\). (Negative \(q\) do not contribute, because we saw earlier ((4.13) and (4.15)) that \(\Delta A = 0\) there.)

5. Conclusion

The seemingly elementary model of a “power wall” has run into several rather profound mathematical problems that are worthy of mathematicians’ attention.

1. What phase shifts \(\delta(p)\) correspond to potentials (or even nonlocal dynamics) qualitatively worthy of being called “soft walls”?
2. What phase shifts do and don’t lead to finite oscillatory integrals (3.25), (3.26), (3.27), (3.28), etc.? When the convergence is unstable, can numerical methods nevertheless be applied to such integrals? Can they be analytically recast into more rapidly convergent integrals?
3. What can one say in general about caustics in the semiclassical solution of time-dependent Schrödinger equations? Are they generically as harmless as in the Mehler formula, or as harmful as in elliptic problems?

Acknowledgments

We thank Gabriel Barton, Lev Kaplan, and Kim Milton for valuable remarks.

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Department of Mathematics, Texas A&M University, College Station, TX, 77845-3368, U.S.A.

E-mail address: jd.bouas@gmail.com (Jeff Bouas)

E-mail address: fulling@math.tamu.edu (Stephen Fulling)

E-mail address: fmera@ucmerced.edu (Fernando Mera)

E-mail address: thapairish@tamu.edu (Krishna Thapa)

E-mail address: cyntrendafilova@gmail.com (Cynthia Trendafilova)

Current address: Department of Physics and Astronomy, University of California – Riverside, 3401 Watkins Dr., Riverside, CA 92521 OK

E-mail address: jeffrey.wagner@ucr.edu (Jef Wagner)