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The local geometric asymptotics of continuum eigenfunction expansions: III. Boundary effects and coefficient singularities

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Abstract. The effect of a boundary condition on the spectral density of a differential operator in one dimension is computed directly from the asymptotic behaviour of the eigenfunctions. From the properly normalised eigenfunction expansion, the contribution of the boundary to the diagonal value of the heat kernel at a point is obtained, and some properties of the special functions arising thereby are derived. A discontinuity, or other singularity, in the coefficient function of the operator is shown to have spectral effects quite analogous to those of a boundary, and the additional effects due to the coexistence of a boundary and a discontinuity are investigated to lowest order.

1. Introduction

This paper's predecessors, I and II (Fulling 1982, 1983), have two main themes. (1) The much studied subject of the asymptotic distribution of the eigenvalues of a differential operator has a generalisation to operators with continuous spectrum, wherein the objects whose asymptotic behaviour is studied are, in the one-dimensional case, the Weyl–Titchmarsh–Kodaira spectral measures at a given point in space. (2) These asymptotics can be related, at least in one dimension, to the high-frequency asymptotics of the eigenfunctions—specifically, the WKB approximation as generalised by Fröman (1966). A more detailed summary of this programme and its motivation has been given by Fulling (1981). The extension to higher dimensions is under investigation, as is the application of the results to the calculation of renormalised observables in quantum field theory with external (e.g., gravitational) potentials.

Before we leave the one-dimensional case, it is instructive to see how our direct approach (in terms of eigenfunction expansions) yields the effect of a *boundary condition* on the asymptotics of spectral measures, and hence on various integral kernels (Green functions) associated with the operator. This paper presents rather detailed information on the principal spectral measure and the heat kernel of a self-adjoint second-order operator on the half-line. (It will be clear how the other spectral measures and other kernels can be similarly calculated should an application warrant.) This constitutes an explicit, detailed demonstration, in the one-dimensional prototype, of phenomena which are known, at least qualitatively, to occur in more general situations. In particular, the notion of a sum over (real) classical paths, in the sense of Balian and Bloch (1971, 1972, 1974), emerges naturally. The methods employed have the charm of being just natural extensions of the techniques of elementary quantum mechanics.

Finally, in the last section the same ideas are applied to differential operators whose coefficients are only piecewise smooth. It is suggested that there is a useful analogy between an *isolated coefficient singularity* and a boundary.

Here is a summary of the content of the body of the paper. Papers I and II were concerned only with asymptotic expansions which are completely determined by the *local* behaviour of the coefficients (symbol) of the operator H under study. Therefore, H was replaced by a 'locally equivalent' operator $\tilde{H}$ which coincides with H near the point x_0 of interest, but whose coefficients trivialise at infinity. The eigenfunction expansion for $\tilde{H}$ was then treated after the fashion of quantum scattering theory. In I and II, x_0 was an interior point, and so the calculations were done for an operator $\tilde{H}$ of the form (2.1) with a potential $V(x)$ of compact support defined on the whole real line. Also, x_0 was a point of smoothness of the original potential, so the new potential was assumed smooth everywhere. In this paper the operator will be defined on an interval with an endpoint at $x=0$, where the Dirichlet, the Neumann, or the most general Robin (2.2) boundary condition is imposed. We pass to a locally equivalent C_0^∞ potential on the half-line $0 \leq x < \infty$, leaving the boundary condition and the potential near the boundary intact, and solve the corresponding scattering problem in the WKB–Fröman approximation. The expansions of the spectral measures, heat kernel, etc, at a point x_0 near the boundary can then be compared with the purely local expansion treated in paper I, where the boundary was ignored. Let us denote the difference between the two expansions by a subscript 'B'.

The picture of such situations which has been built up by several decades of research is the following, when specialised to the case at hand. The boundary correction $d\mu_B^{jk}(\lambda; x)$ to a spectral measure does not necessarily become small as the eigenparameter λ approaches infinity, even if x is far from the boundary. That is, the local expansion is *not* an asymptotic approximation, in the technical sense, to the true spectral measure. However, $d\mu_B^{jk}$, as a function of λ, exhibits oscillations whose frequency increases with x. These oscillations cause many integrals with respect to $d\mu_B^{jk}$ to be rapidly decreasing functions of x. Thus, for example, the boundary correction to the heat kernel, $K_B(t, x, x)$, is heavily concentrated near the boundary if t is small. At any interior point x, the local (boundary-free) expansion of $K(t, x, x)$ is genuinely asymptotic, to any order in t. However, this expansion is not uniform in x, and hence to get a valid approximation to the integral of $K(t, x, x)$ over any interval with 0 as an endpoint it is necessary to include the integral of K_B, which makes a finite-order contribution. Related remarks apply to the vacuum energy density of a quantised field near boundaries (Deutsch and Candelas 1979, Kennedy *et al* 1980). This behaviour is prototypical of the difference between the spectral asymptotics of two locally equivalent operators.

All these features show up quite explicitly in the calculations presented in §§ 2 and 3. (The treatment is not entirely self-contained, since at one point we must appeal to the independently established local validity of the heat-kernel expansion to fix some constants of integration.) In § 2 we derive the formula (2.18) for $d\mu_B^{00}(\lambda, x)$ in terms of the amplitude at x of the scattering wavefunction for energy λ. This is expanded as a power series (2.25) in both $\lambda^{-1/2}$ and x, with 'geometrical' coefficients determined by the Robin constant and the behaviour of the potential right at the boundary. In § 3, (2.25) is used to compute $K_B(t, x, x)$ (3.7) and its integral over x (3.10). The latter is a power series in $t^{1/2}$, which agrees numerically with known results (Gilkey 1979). The former must be expressed in terms of certain transcendental functions which generalise the incomplete gamma function. Their properties, including limiting behaviour for large and small argument, are investigated in theorem 3.1.

Section 4 raises the question of what happens when $V(x)$ is not smooth. An isolated coefficient singularity has spectral effects similar to those of a boundary, because it causes non-trivial reflection amplitudes in the eigenfunctions. We consider the case of a finite jump discontinuity in V or one of its derivatives, because it can be treated by a simple extension of the previous methods. Like the boundary, the jump contributes oscillations to the spectral measure everywhere, with frequency proportional to the distance from the jump, and these oscillations produce in the heat kernel, etc, an extra term which is significantly large over a finite neighbourhood of the jump and dies off rapidly with distance from it. Finally, the combined effect of a jump and a boundary is compared, to lowest order in ω^{-1}, with the separate effects of the two elements.

2. Spectral measures near the boundary

Consider a differential operator of the form

$$H = -(\mathrm{d}^2/\mathrm{d}x^2) + V(x) \tag{2.1}$$

where V is smooth (C^∞), $V(x) = 0$ for x sufficiently large, and $V(x)$ tends to a finite limit as $x \to 0$. Then $x = 0$ is a regular endpoint in the sense of Sturm–Liouville theory, and $x = \infty$ is a singular endpoint of the limit-point type. The boundary condition

$$\psi'(0) = \kappa\psi(0) \tag{2.2}$$

for some $\kappa \in \mathbb{R}$ makes H essentially self-adjoint (and bounded below) on the domain of all C^∞ functions ψ satisfying (2.2) and vanishing at large x (see, e.g., Reed and Simon 1975). The Neumann boundary condition is the case $\kappa = 0$. The Dirichlet condition

$$\psi(0) = 0 \tag{2.3}$$

may be thought of as the limiting case $\kappa = +\infty$, but will be treated separately in our computations.

The general classical solution of the differential equation

$$H\psi_p = \lambda\psi_p \qquad \lambda = \omega^2 \qquad \omega = |p| \tag{2.4}$$

has for large λ the WKB–Fröman expansion

$$\psi_p(x) \sim Y_p(x)^{-1/2} \exp\left(\mathrm{i}p \int_{x_0}^{x} Y_p(x')\,\mathrm{d}x'\right) \tag{2.5a}$$

$$Y_p(x) \equiv \sum_{n=0}^{\infty} p^{-2n} Y_{2n}(x) \tag{2.5b}$$

or a linear combination of these for the two possible signs of p. Under the given conditions on V, this expansion is uniform in x. With the usual normalisation, one has

$$Y_0 = 1 \qquad Y_2 = -\tfrac{1}{2}V \qquad Y_4 = \tfrac{1}{8}(V'' - V^2) \tag{2.6}$$

etc (see theorem 4.1 of I).

We choose the arbitrary starting point x_0 in (2.5) to be the point at which the spectral measures (Kodaira 1949, Titchmarsh 1962) are to be evaluated. The latter are defined, as in I, by

$$\mathrm{d}E_\lambda(x, y) = \sum_{j,k=0}^{1} \psi_{\lambda j}(x)\, \mathrm{d}\mu^{jk}(\lambda\,; x_0)\overline{\psi_{\lambda k}(y)} \tag{2.7}$$

where $\mathrm{d}E_\lambda(x, y)$ is the differential of the kernel (Gårding 1954) of the projection operators in the spectral decomposition

$$H = \int_{-\infty}^{\infty} \lambda\, \mathrm{d}E_\lambda \tag{2.8}$$

and $\psi_{\lambda 0}$ and $\psi_{\lambda 1}$ are the solutions of (2.4) satisfying

$$\psi_{\lambda j}^{(k)}(x_0) = \delta_j^k. \tag{2.9}$$

(Under our assumptions on V, the spectrum is continuous at large λ and hence we expect $\mathrm{d}E_\lambda(x, y)/\mathrm{d}\lambda$ to make sense as a *function* of λ.)

By analogy to (4.6) of I, we determine $\mathrm{d}\mu^{jk}$ (asymptotically) by equating (2.7) to an alternative representation of $\mathrm{d}E_\lambda(x, y)$ which is completely known. Attention may be restricted to $\lambda > 0$. Let $\phi_\omega(x)$ be the solution of (2.4) which satisfies the boundary condition (2.2) (or (2.3)) defining H and is normalised so that

$$\phi_\omega(x) \sim \sin(\omega x + \delta) \qquad \text{as } x \to \infty \tag{2.10}$$

(where δ depends on κ and ω). Only solutions of (2.4) proportional to ϕ_ω may appear in the eigenfunction expansion associated with H. It is well known that the functions $\{(2/\pi)^{1/2}\phi_\omega(x)\colon \omega > 0\}$ are orthonormal in the sense of the Dirac delta in the variable ω. From these two facts it follows that

$$\mathrm{d}E_\lambda(x, y) = 2\pi^{-1}\phi_\omega(x)\overline{\phi_\omega(y)}\, \mathrm{d}\omega \tag{2.11}$$

(Kodaira 1949).

Obtaining $\mathrm{d}\mu^{00}(\lambda\,; x_0)$ from (2.7) and (2.11) amounts to calculating $|\phi_\omega(x_0)|^2$. Therefore, we express ϕ_ω (for large ω) in terms of a basis of solutions with the WKBF behaviour (2.5):

$$\phi_\omega = A_\omega \psi_\omega + B_\omega \psi_{-\omega}. \tag{2.12}$$

A_ω and B_ω are determined by the two boundary conditions, (2.2) and (2.10). Recall (Fröman 1966, Fulling 1983) that the WKBF functions satisfy

$$\psi'_p \sim \mathrm{i}pN_p\psi_p, \tag{2.13}$$

where

$$Y_p = \operatorname{Re} N_p = \tfrac{1}{2}(N_p + N_{-p}) = Y_\omega \tag{2.14a}$$

is the series (2.5*b*), and

$$\operatorname{Im} N_p = \frac{1}{2\mathrm{i}}(N_p - N_{-p}) = \frac{1}{2p}\frac{\mathrm{d}}{\mathrm{d}x}\ln Y_\omega. \tag{2.14b}$$

Thus, in the asymptotic limit,

$$\phi'_\omega = A_\omega \mathrm{i}\omega N_\omega \psi_\omega - B_\omega \mathrm{i}\omega N_{-\omega}\psi_{-\omega}. \tag{2.15}$$

The Robin boundary condition (2.2) becomes

$$A_\omega(\kappa - \mathrm{i}\omega N_\omega)\psi_\omega(0) + B_\omega(\kappa + \mathrm{i}\omega N_{-\omega})\psi_{-\omega}(0) = 0$$

or

$$\frac{A_\omega}{B_\omega} = -\frac{\kappa + \mathrm{i}\omega\overline{N_\omega(0)}}{\kappa - \mathrm{i}\omega N_\omega(0)} \exp\left(2\mathrm{i}\omega \int_0^{x_0} Y_\omega(x')\,\mathrm{d}x'\right) \equiv \zeta_\omega(x_0). \qquad (2.16)$$

On the other hand, comparing (2.10) with (2.12) and (2.5) (where $Y_\omega = 1$ at sufficiently large x), one sees that

$$|A_\omega| = \tfrac{1}{2} = |B_\omega|. \qquad (2.17)$$

These last two equations are consistent and determine A_ω and B_ω up to an irrelevant overall phase. (These, and similar results, are valid modulo terms of some arbitrarily high order in ω^{-1}, determined by the order at which the (divergent) series Y in (2.5) is truncated; beyond that order A_ω and B_ω should not even be regarded as well defined.) For the Dirichlet problem (2.3), ζ_ω is given by (2.16) with the fractional prefactor omitted, as one would have guessed by taking $\kappa \to \infty$.

Set $x = y = x_0$ in (2.7) and successively use (2.9) and (2.11), (2.12) and (2.5), (2.16) and (2.17), and $|\zeta_\omega| = 1$:

$$\begin{aligned}
\mathrm{d}\mu^{00}(\lambda; x) &= 2\pi^{-1}|\phi_\omega(x)|^2\,\mathrm{d}\omega \\
&= 2\pi^{-1}|A_\omega Y_\omega(x)^{-1/2} + B_\omega Y_{-\omega}(x)^{-1/2}|^2\,\mathrm{d}\omega \\
&= (2\pi)^{-1} Y_\omega(x)^{-1}|1 + \zeta_\omega(x)|^2\,\mathrm{d}\omega \\
&= \pi^{-1} Y_\omega(x)^{-1}(1 + \mathrm{Re}\,\zeta_\omega(x))\,\mathrm{d}\omega.
\end{aligned}$$

If $\zeta_\omega(x)$ were 0, this would be the formula valid when M is the whole real line and $V \in C_0^\infty(\mathbb{R})$; see (4.7) and (4.9) of I. *Hence the difference between* $\mathrm{d}\mu^{00}$ *with boundary and* $\mathrm{d}\mu^{00}$ *without boundary is*

$$\mathrm{d}\mu_{\mathrm{B}}^{00}(\lambda; x) = \pi^{-1} Y_\omega(x)^{-1}\,\mathrm{Re}\,\zeta_\omega(x)\,\mathrm{d}\omega. \qquad (2.18)$$

This is our main result. Here ζ is defined by (2.16) (with (2.14)), while Y is the same as in I and is described in (2.5) and (2.6) of the present paper. Formulae for $\mathrm{d}\mu_{\mathrm{B}}^{01} = \mathrm{d}\mu_{\mathrm{B}}^{10}$ and $\mathrm{d}\mu_{\mathrm{B}}^{11}$ could be obtained similarly, using (2.7), (2.9) and (2.11)–(2.13).

The qualitative behaviour of

$$\rho_{\mathrm{B}}^{00}(\omega; x) \equiv \pi\,\mathrm{d}\mu_{\mathrm{B}}^{00}(\omega; x)/\mathrm{d}\omega \qquad (2.19)$$

is instructive. It is an oscillatory function, whose amplitude does *not* become small as $\omega \to \infty$ or as $x \to \infty$. However, the period of the oscillations with respect to one of these variables tends to zero as the other variable, regarded as a parameter, approaches infinity. These observations are consistent with the general situation described in I. Consider an operator $\tilde{H}$ defined on the whole line, whose potential $\tilde{V} \in C_0^\infty(\mathbb{R})$ coincides with V in a neighbourhood of x. (One says that H and $\tilde{H}$ are 'locally equivalent'.) The asymptotic expansion of the ρ^{00} of $\tilde{H}$, derived in I, is not asymptotic to the ρ^{00} of H, because the remainder is dominated by ρ_{B}^{00}, which does not decrease rapidly. Nevertheless, if one stays far enough away from the boundary, $\rho_{\mathrm{B}}^{00}(\omega; x)$ will oscillate so fast that it will make an insignificant contribution to an integral $\int f(\omega)\rho^{00}(\omega; x)\,\mathrm{d}\omega$ if f is a sufficiently slowly varying function. (This must be made more precise in the context of any particular application, either by hard analysis of the integrals or, more likely, by an *a priori* proof, as in Greiner (1971) or Fulling *et al* (1981), that the object being calculated is completely determined by the local behaviour of V.) Similarly, the detailed behaviour of $\rho_{\mathrm{B}}^{00}(\omega; x)$ at large ω should be invisible in a quantity that involves a 'smearing' in x over a distance scale large compared with the wavelength, $2\pi\omega^{-1}$.

Remark 2.1. For fixed x, the angular frequency of oscillation of $\rho_{\mathrm{B}}^{00}(\omega)$ is, to lowest order, $2x$ (see formulae below). For operators H with discrete spectra, it is known that, roughly speaking, the asymptotic density of eigenvalues manifests oscillations with frequencies equal to the lengths of any periodic orbits of the classical-mechanical system whose Hamiltonian is the principal symbol of H, with specular reflection at the boundary (see Balian and Bloch 1972, Duistermaat and Guillemin 1975 and the work of Colin de Verdière and Chazarain referenced in the latter). Our result suggests that the 'local' version of this principle is the following: $\mathrm{d}E_{\omega^2}(x, x)$ *exhibits oscillations (as a function of* ω*) with frequencies equal to the lengths of any classical paths which start and end at* x *(not necessarily with initial and final directions of motion the same).* Better approximations to the effective frequency of oscillation can be obtained by keeping higher-order terms in the series $Y_\omega(x')$ in (2.16). In particular, since (Campbell 1972) the coefficient of V^n in Y_{2n} is

$$\frac{-(2n)!}{2^{2n}(n!)^2(2n-1)} = -\frac{(2n-3)!!}{2^n n!} = (-1)^n \binom{\frac{1}{2}}{n}$$

all the terms in Y which do not involve derivatives of V can be summed to yield $(1-\omega^{-2}V)^{1/2}$. (This is the leading term of a semiclassical expansion in the sense of Wilk *et al* (1981) and Fujiwara *et al* (1982).) In this approximation the exponential factor in (2.16) becomes

$$\exp\left(\mathrm{i}\int_0^{x_0} 2(\omega^2 - V(x'))^{1/2}\,\mathrm{d}x'\right). \tag{2.20}$$

The integral here can be interpreted (cf Balian and Bloch 1971, § II.A) as the action (Hamilton's *characteristic* function) of the trajectory from x to the boundary and back, traversed by a particle with energy ω^2. The derivative of the integral with respect to ω can be regarded as the effective frequency of oscillation of $\rho_{\mathrm{B}}^{00}(\omega)$. Again there is a close parallel in the case of discrete spectrum: The well known WKB formula (Messiah 1961, (VI.54)) implicitly determining the Nth eigenvalue (giving N as a function of ω_N^2) involves the same integrand, but the integral is extended over the entire orbit of a bound classical particle. The derivative of N approximates the reciprocal of the spacing between eigenvalues, and hence is an oscillation frequency of the eigenvalue density.

Let us investigate ρ_{B}^{00} in more detail, by isolating the leading oscillatory factor and expanding the rest in negative powers of ω. The factor Y^{-1} in (2.18) is simply equal to the boundary-free ρ^{00}, and its expansion has been given in (4.10) of I (where $E = -V$); it begins

$$Y(x)^{-1} \sim 1 + \tfrac{1}{2}V(x)\omega^{-2} + \tfrac{1}{8}(-V''(x) + 3V(x)^2)\omega^{-4} + \mathrm{O}(\omega^{-6}). \tag{2.21}$$

For fixed $K \neq \infty$, the prefactor in (2.16) is found to have the expansion

$$\frac{\kappa + \mathrm{i}\omega\overline{N_\omega(0)}}{\kappa - \mathrm{i}\omega N_\omega(0)} \sim -[1 - 2\mathrm{i}\kappa\omega^{-1} - 2\kappa^2\omega^{-2} + \mathrm{i}(\tfrac{1}{2}V'(0) - \kappa V(0) + 2\kappa^3)\omega^{-3} + \mathrm{O}(\omega^{-4})]. \tag{2.22}$$

(The expansion of N is taken from II, or obtained from (2.14).) The rest of (2.16) is

$$-\exp\left(2\mathrm{i}\,\omega\int_0^x Y(x')\,\mathrm{d}x'\right)$$
$$\sim -\mathrm{e}^{2\mathrm{i}\omega x}\sum_{m=0}^{\infty}\frac{1}{m!}\left(2\mathrm{i}\sum_{n=1}^{\infty}\omega^{1-2n}\int_0^x Y_{2n}(x')\,\mathrm{d}x'\right)^m$$
$$= -\mathrm{e}^{2\mathrm{i}\omega x}\left\{1+2\mathrm{i}\omega^{-1}\int Y_2-2\omega^{-2}\left(\int Y_2\right)^2\right.$$
$$\left.+\mathrm{i}\omega^{-3}\left[2\int Y_4-\tfrac{4}{3}\left(\int Y_2\right)^3\right]+\mathrm{O}(\omega^{-4})\right\}. \tag{2.23}$$

Multiplying (2.21) and (2.23), one obtains

ρ_{B}^{00}(Dirichlet)

$$\sim -\mathrm{Re}\left(\mathrm{e}^{2\mathrm{i}\omega x}\left\{1+2\mathrm{i}\omega^{-1}\int Y_2+\omega^{-2}\left[\tfrac{1}{2}V(x)-2\left(\int Y_2\right)^2\right]\right.\right.$$
$$+\mathrm{i}\omega^{-3}\left[V(x)\int Y_2+2\int Y_4-\tfrac{4}{3}\left(\int Y_2\right)^3\right]$$
$$\left.\left.+\tfrac{1}{8}\omega^{-4}(-V''(x)+3V(x)^2+\mathrm{O}(x))+\mathrm{O}(\omega^{-5})\right\}\right) \tag{2.24a}$$

(where an abbreviated notation for integrals from 0 to x is used). The formula for the Robin case is obtained by multiplying by (2.22) before taking the real part:

$$\rho_{\mathrm{B}}^{00}\sim\mathrm{Re}\left(\mathrm{e}^{2\mathrm{i}\omega x}\left\{1+\mathrm{i}\omega^{-1}\left(2\int Y_2-2\kappa\right)\right.\right.$$
$$+\omega^{-2}\left[\tfrac{1}{2}V(x)-2\left(\int Y_2\right)^2+4\kappa\int Y_2-2\kappa^2\right]$$
$$+\mathrm{i}\omega^{-3}\left[V(x)\int Y_2+2\int Y_4-\tfrac{4}{3}\left(\int Y_2\right)^3-\kappa V(x)\right.$$
$$\left.\left.\left.+4\kappa\left(\int Y_2\right)^2-4\kappa^2\int Y_2-\tfrac{1}{2}V'(0)-\kappa V(0)+2\kappa^3\right]+\mathrm{O}(\omega^{-4})\right\}\right). \tag{2.24b}$$

Since ordinarily ρ_{B}^{00} is of practical importance only near the boundary, and expansion (2.23) is already non-uniform in x, it is natural to make a further expansion in powers of x. This yields series whose coefficients are dimensionally homogeneous polynomial functionals of κ and V on the boundary:

$$\rho_{\mathrm{B}}^{00}(\omega;x)\sim\mathrm{Re}\left(\mathrm{e}^{2\mathrm{i}\omega x}\sum_{n=0}^{\infty}\sum_{p=0}^{n}\rho_{\mathrm{B}np}^{00}\omega^{-p}x^{n-p}\right). \tag{2.25}$$

For the Dirichlet case the first few coefficients are

$$\begin{aligned}
&\rho_{\mathrm{B}00}^{00}=-1 \qquad \rho_{\mathrm{B}1p}^{00}=(0,0)\\
&\rho_{\mathrm{B}2p}^{00}=(0,\mathrm{i}V,-\tfrac{1}{2}V) \qquad \rho_{\mathrm{B}3p}^{00}=(0,\tfrac{1}{2}\mathrm{i}V',-\tfrac{1}{2}V',0)\\
&\rho_{\mathrm{B}40}^{00}=0 \qquad \rho_{\mathrm{B}41}^{00}=\tfrac{1}{6}\mathrm{i}V'' \qquad \rho_{\mathrm{B}42}^{00}=-\tfrac{1}{4}V''+\tfrac{1}{2}V^2\\
&\rho_{\mathrm{B}43}^{00}=-\tfrac{1}{4}\mathrm{i}(V''-3V^2) \qquad \rho_{\mathrm{B}44}^{00}=\tfrac{1}{8}(V''-3V^2).
\end{aligned} \tag{2.26a}$$

Here V and its derivatives are evaluated at 0. For the Neumann–Robin problems only the terms up to $n=3$ are listed, since to find $\rho^{00}_{\mathrm{B}44}$ one would need one more term in (2.22):

$$\begin{aligned}&\rho^{00}_{\mathrm{B}00}=1 \qquad \rho^{00}_{\mathrm{B}1p}=(0,\,-2\mathrm{i}\kappa)\\ &\rho^{00}_{\mathrm{B}2p}=(0,\,-\mathrm{i}V,\tfrac{1}{2}V-2\kappa^2)\\ &\rho^{00}_{\mathrm{B}30}=0 \qquad \rho^{00}_{\mathrm{B}31}=-\tfrac{1}{2}\mathrm{i}V'\\ &\rho^{00}_{\mathrm{B}32}=\tfrac{1}{2}V'-2\kappa V \qquad \rho^{00}_{\mathrm{B}33}=\mathrm{i}(\tfrac{1}{2}V'-2\kappa V+2\kappa^3).\end{aligned}\tag{2.26b}$$

Obviously, similar expansions for ρ^{01}_{B} and ρ^{11}_{B} could be derived. The coefficients $\rho^{jk}_{\mathrm{B}np}[\kappa, V]$ are the fundamental 'spectral invariants' which determine the behaviour of Green functions, etc, of H near the boundary. For example, from their analogues in higher dimensions it should be possible to reproduce the results of Deutsch and Candelas (1979) and Kennedy *et al* (1980) for the singular behaviour of the energy density of a quantised field near a boundary.

Remark 2.2. $\rho^{00}_{\mathrm{B}np}$ is of order n, if the order of a monomial in κ and derivatives of V is defined as the sum of

(i) the degree in κ,
(ii) twice the degree in V (and its derivatives),
(iii) the total number of differentiations.

Remark 2.3. $\rho^{00}_{\mathrm{B}np}$ is real if p is even, pure imaginary if p is odd. Also, $\rho^{00}_{\mathrm{B}n0}=0$ except for $\rho^{00}_{\mathrm{B}00}=\pm 1$.

Remark 2.4. In expanding the spectral density in powers of ω^{-1}, we have committed willy-nilly an expansion in κ. That is, we are treating the Robin boundary condition by perturbation about the Neumann case. This is also true of the standard expansion (3.8) of the heat kernel in powers of t. Balian and Bloch (1970) have emphasised that for some applications it is not appropriate to assume that κ is small. Rather, one may need an expansion which is uniform in κ. (The same argument can be made for the potential V, leading to a 'semiclassical' expansion (Wilk *et al* 1981, Fujiwara *et al* 1982), where the order of a term is determined only by the number of differentiations.) In the present framework, such an expansion is obtained by treating $1+\mathrm{i}\kappa\omega^{-1}$ as a quantity of order unity in expanding ζ_ω; thus (2.22) is replaced by

$$\frac{\kappa+\mathrm{i}\omega\overline{N_\omega(0)}}{\kappa-\mathrm{i}\omega N_\omega(0)}\sim\frac{\omega^2-\kappa^2-2\mathrm{i}\kappa\omega}{\omega^2+\kappa^2}\left(-1+\frac{\mathrm{i}\kappa\omega}{\omega^2+\kappa^2}V(0)\omega^{-2}+\mathrm{O}(\omega^{-3})\right)$$

and the ω-dependent coeffiicients in this series are carried intact into the new versions of (2.24b) and (2.26b). As $\kappa\to+\infty$ the results will go over smoothly into the formulae for the Dirichlet problem, so the latter no longer appears as such a singular case. Unfortunately, with such complicated expressions it is unlikely that calculations parallel to § 3 (for instance) can be carried out in closed form.

3. Heat kernel near the boundary

As an explicit example of the significance of the expansion of ρ^{00}_{B}, let us compute the boundary correction to the heat kernel, $K(t,x,y)$, on the diagonal $(x=y)$. Recall

(I, (3.2)) that

$$K(t, x, x) = \int_{-\infty}^{\infty} e^{-\lambda t}\, d\mu^{00}(\lambda\,;x). \tag{3.1}$$

Thus

$$K_B(t, x, x) \sim \pi^{-1} \int^{\infty} e^{-\omega^2 t} \rho_B^{00}(\omega\,; x)\, d\omega \tag{3.2}$$

is the boundary correction to the small-t asymptotic form of $K(t, x, x)$. The contribution from $d\mu^{00}(\lambda, x)$ at small λ (i.e., $-\infty < \lambda < A$, $A > 0$ arbitrary) is an analytic function of t, and our initial calculations will be meaningful only modulo such terms. We confine our attention to the situation described at the beginning of § 2, in which the spectral expansion (2.25) is rigorously asymptotic; it would also be possible, along the lines of I, § 3, to discuss the more general case (unbounded V, a finite interval M, etc) where the correspondence between the coefficients in the two series is more formal. Since the asymptotic validity of the resulting expansion of the heat kernel is not in doubt, complete justification of the estimates on the remainder terms in the intermediate steps will not be provided.

It would be convenient to place the lower limit of integration in (3.2) at $\omega = 0$, were it not for the negative powers of ω in the integrand, (2.25). As in I, we circumvent this spurious divergence by studying

$$\left(-\frac{\partial}{\partial t}\right)^m K_B(t, x, x) \sim \frac{1}{\pi} \int^{\infty} e^{-\omega^2 t} \omega^{2m} \rho_B^{00}(\omega\,; x)\, dx \tag{3.3}$$

and truncating the series (2.25) while $2m - p + 1$ is still positive. The integrals which are then needed are (Gradshteyn and Ryzhik 1965, (3.896.4) and (3.952.1))

$$\begin{aligned} \int_0^{\infty} e^{-\omega^2 t} \cos 2\omega x\, d\omega &= \tfrac{1}{2}\pi^{1/2} t^{-1/2}\, e^{-x^2/t} \\ \int_0^{\infty} \omega\, e^{-\omega^2 t} \sin 2\omega x\, d\omega &= \tfrac{1}{2}\pi^{1/2} x t^{-3/2}\, e^{-x^2/t}. \end{aligned} \tag{3.4}$$

From (2.25) with remark 2.3 we obtain

$$K_B(t, x, x) = \tfrac{1}{2}\pi^{-1/2} t^{-1/2}\, e^{-x^2/t} \rho_{B00}^{00} + O(\ln t) \tag{3.5a}$$

$$\begin{aligned} -\partial K_B/\partial t = {} & -\partial(3.5a)/\partial t + \tfrac{1}{2}i\pi^{-1/2} t^{-3/2}\, e^{-x^2/t}\left(\sum_{n=1}^{4} x^n \rho_{Bn1}^{00} + O(x^5)\right) \\ & + \tfrac{1}{2}\pi^{-1/2} t^{-1/2}\, e^{-x^2/t}\left(\sum_{n=2}^{4} x^{n-2} \rho_{Bn2}^{00} + O(x^3)\right) + O(\ln t) \end{aligned} \tag{3.5b}$$

$$\begin{aligned} \partial^2 K_B/\partial t^2 = {} & -\partial(3.5b)/\partial t + \tfrac{1}{2}i\pi^{-1/2} t^{-3/2}\, e^{-x^2/t}\left(\sum_{n=3}^{4} x^{n-2} \rho_{Bn3}^{00} + O(x^3)\right) \\ & + \tfrac{1}{2}\pi^{-1/2} t^{-1/2}\, e^{-x^2/t}(\rho_{B44}^{00} + O(x)) + O(\ln t). \end{aligned} \tag{3.5c}$$

In each bracketed expression, all terms of order four or less in the sense of remark 2.2 have been kept.

Define

$$I_{0,q}(x,t)=t^{-q/2}\,e^{-x^2/t} \tag{3.6a}$$

$$I_{m,q}(x,t)=\int_0^t I_{m-1,q}(x,t')\,dt'. \tag{3.6b}$$

Then from (3.5) we have

$$\begin{aligned}2\pi^{1/2}K_B(t,x,x)&=I_{0,1}(x,t)\rho^{00}_{B00}-iI_{1,3}(x,t)\Big(\sum_{n=1}^{4}x^n\rho^{00}_{Bn1}+O(x^5)\Big)\\&\quad-I_{1,1}(x,t)\Big(\sum_{n=2}^{4}x^{n-2}\rho^{00}_{Bn2}+O(x^3)\Big)+iI_{2,3}(x,t)\Big(\sum_{n=3}^{4}x^{n-2}\rho^{00}_{Bn3}+O(x^3)\Big)\\&\quad+I_{2,1}(x,t)(\rho^{00}_{B44}+O(x))+C_1(x)+C_2(x)t+O(t^2\ln t).\end{aligned} \tag{3.7}$$

For fixed $x\neq 0$, $K_B(t,x,x)$ must vanish faster than any power as $t\to 0$, since the local heat-kernel expansion constructed without reference to a boundary is a valid parametrix there (see I, theorem 3.2). This property is possessed by the $I_{m,q}$ (see theorem below), but not by the terms containing C_1 and C_2 unless they vanish, which, therefore, they must do. This appeal to prior knowledge of the structure of the heat kernel compensates for our ignorance of μ^{00}_B at small λ.

Let us establish and verify, through the first few orders, the relationship between the ρ^{jk}_{Bnp} coefficients and the spectral invariants in the well known expansion

$$\int_0^\varepsilon K_B(t,x,x)\,dx\sim\sum_{n=0}^{\infty}t^{n/2}E^B_{n/2}(0,H), \tag{3.8}$$

where ε is sufficiently large compared with $t^{1/2}$ (Gilkey 1979, § 3). (In higher dimensions this integral is still one dimensional and defines a function on the boundary of M.) Since the integrand falls off very rapidly with x, this integration can be interchanged with the summations and t' integrations in (3.7) and (3.6b) and the upper limit can be taken to ∞. Using

$$\int_0^\infty x^n\,e^{-x^2/t}\,dx=\begin{cases}\pi^{1/2}2^{-1-n/2}(n-1)!!\,t^{(n+1)/2} & \text{for } n \text{ even}\\ \frac{1}{2}[\frac{1}{2}(n-1)]!\,t^{(n+1)/2} & \text{for } n \text{ odd}\end{cases} \tag{3.9}$$

one obtains

$$\begin{aligned}\int_0^\infty K_B(t,x,x)\,dx&=\tfrac{1}{4}\rho^{00}_{B00}-i(4\pi)^{-1/2}\rho^{00}_{B11}t^{1/2}-\tfrac{1}{8}(i\rho^{00}_{B21}+2\rho^{00}_{B22})t\\&\quad-\tfrac{1}{3}(4\pi)^{-1/2}(i\rho^{00}_{B31}+\rho^{00}_{B32}-2i\rho^{00}_{B33})t^{3/2}\\&\quad+\tfrac{1}{32}(-3i\rho^{00}_{B41}-2\rho^{00}_{B42}+2i\rho^{0}_{B43}+4\rho^{00}_{B44})t^2+O(t^{5/2}).\end{aligned} \tag{3.10}$$

Substituting values of the coefficients from (2.26), one has for the Dirichlet problem

$$\begin{aligned}&E^B_0=-\tfrac{1}{4} \qquad E^B_{1/2}=0 \qquad E^B_1=\tfrac{1}{4}V\\&E^B_{3/2}=(4\pi)^{-1/2}\tfrac{1}{3}V' \qquad E^B_2=\tfrac{1}{16}(V''-V^2)\end{aligned} \tag{3.11a}$$

and for the Neumann–Robin case

$$E_0^{\mathrm{B}}=\tfrac{1}{4} \qquad E_{1/2}^{\mathrm{B}}=(4\pi)^{-1/2}(-2\kappa)$$
$$E_1^{\mathrm{B}}=\tfrac{1}{4}(-V+2\kappa^2) \qquad E_{3/2}^{\mathrm{B}}=(4\pi)^{-1/2}\,\tfrac{2}{3}(-V'+3\kappa V-2\kappa^3) \tag{3.11b}$$

in agreement with Gilkey (1979, theorem 3.4), where the notation is $S=-\kappa$, $\mathscr{E}=-V$.

In conclusion, we investigate in detail the functions $I_{m,q}$ which appear in (3.6) and (3.7). (We are primarily interested in q an odd integer.)

Lemma 3.1. $I_{1,q}$ can be expressed in terms of the incomplete gamma function (Gradshteyn and Ryzhik 1965, § 8.35):

$$I_{1,q}(x,t)=x^{2-q}\Gamma(\tfrac{1}{2}q-1,x^2/t). \tag{3.12}$$

Proof. Let

$$\alpha=\tfrac{1}{2}q-1 \qquad y=x^2/t \qquad y'=x^2/t'. \tag{3.13}$$

Then

$$I_{1,q}(x,t)\equiv\int_0^t (t')^{-q/2}\,\mathrm{e}^{-x^2/t'}\,\mathrm{d}t'$$
$$=x^{2-q}\int_y^\infty y^{\alpha-1}\,\mathrm{e}^{-y}\,\mathrm{d}y\equiv x^{2-q}\Gamma(\alpha,y).$$

Lemma 3.2. $x^{q-2m}I_{m,q}(x,tx^2)$ is independent of x.

This is easily established from the definition (3.6) by induction on m.

Theorem 3.1. Let $I_{m,q}$ $(m=0,1,2,\ldots)$ be defined by (3.6). Then

(i) For $m\geqslant 1$, the $I_{m,q}$ satisfy

$$I_{m,q+2}(x,t)=x^{-2}((\tfrac{1}{2}q-1)I_{m,q}(x,t)+I_{m-1,q-2}(x,t)). \tag{3.14}$$

(ii) In the limit $t\ll x^2$, there is an asymptotic expansion of the form

$$I_{m,q}(x,t)\sim x^{-2m}t^{2m-q/2}\,\mathrm{e}^{-x^2/t}\left(1+\sum_{n=1}^{\infty}a_n(x^2/t)^{-n}\right). \tag{3.15}$$

(iii) For $q\neq 2,0,-2,-4,\ldots$, there exist numbers $\tilde{\Gamma}_m(q)$ such that

(a) $\tilde{\Gamma}_0(q)=0$;

(b) for $m\geqslant 1$,

$$\tilde{\Gamma}_m(q+2)-(\tfrac{1}{2}q-1)\tilde{\Gamma}_m(q)-\tilde{\Gamma}_{m-1}(q-2)=0; \tag{3.16}$$

(c) if $m\geqslant 1$ and $q>2m$,

$$\tilde{\Gamma}_m(q)=\int_0^\infty\left(I_{m-1,q}(1,t)-\sum_{b=1}^{m-1}\tilde{\Gamma}_b(q)\frac{t^{m-1-b}}{(m-1-b)!}\right)\mathrm{d}t. \tag{3.17}$$

(In particular, $\tilde{\Gamma}_1(q)=\Gamma(\tfrac{1}{2}q-1)$.) For $q\neq 2,0,-2,\ldots$, $I_{m,q}$ is given by

$$I_{m,q}(x,t)=\sum_{b=1}^{m}\frac{\tilde{\Gamma}_b(q)}{(m-b)!}x^{2b-q}t^{m-b}+(-1)^m t^{m-q/2}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(\tfrac{1}{2}q+n-m)}{\Gamma(\tfrac{1}{2}q+n)}(x^2/t)^n. \tag{3.18}$$

(The second term is an entire function of x^2.) Therefore, in the limit $x \ll t^{1/2}$, if $q<2$ or $m=0$ the dominant term is the constant term, $(-1)^m t^{m-q/2}\Gamma(\frac{1}{2}q-m)/\Gamma(\frac{1}{2}q)$, whereas if $q>2$ and $m \geqslant 1$ the dominant term is $\Gamma(\frac{1}{2}-1)x^{2-q}t^{m-1}$.

The statements in the theorem generalise known properties of the incomplete and complete gamma functions. In its proof we shall occasionally use the notations (3.13).

Proof of (i) and (ii). If $m=1$, then (i) is equivalent by lemma 1 to

$$\Gamma(\alpha+1, y)=\alpha\Gamma(\alpha, y)+y^\alpha \mathrm{e}^{-y}$$

(Gradshteyn and Ryzhik 1965, (8.356.2)), which is established by an obvious integration by parts. For $m>1$ the relation follows immediately by integration. It is obvious from the definition that

$$x^{-2p}I_{m,q}(x, t)/I_{m,q-2p}(x, t)=\mathrm{O}(y^{-p}).$$

Hence iterating (i) in q yields an asymptotic series

$$I_{m,q}(x, t)=x^{-2}I_{m-1,q-4}+x^{-4}(\alpha-1)I_{m-1,q-6}+\ldots.$$

Iterating this result in m, one eventually reaches a series of powers of y^{-1}, times e^{-y}. For example,

$$\begin{aligned}I_{2,q}&=x^{-2}\{x^{-2}I_{0,q-8}+x^{-4}[\tfrac{1}{2}(q-4)-2]I_{0,q-10}+\ldots\}+x^{-4}(\tfrac{1}{2}q-2)(x^{-2}I_{0,q-10}+\ldots)+\ldots\\&=x^{-4}t^{4-q/2}\mathrm{e}^{-y}[1+(q-6)y^{-1}+\mathrm{O}(y^{-2})].\end{aligned}$$

In general, the leading term is

$$I_{m,q}\sim x^{-4}I_{m-2,q-8}\sim\ldots\sim x^{-2m}I_{0,q-4m}=x^{-2m}t^{2m-q/2}\mathrm{e}^{-y}.$$

Proof of (iii). For $m=0$, (3.18) is the power series of the entire function $I_{0,q}=t^{-q/2}\mathrm{e}^{-y}$, and the other statements are vacuous. We assume all the statements for $m-1$ and prove them for m. By virtue of (3.18), the integral in (3.17) converges (at the upper limit) if $q>2m$. Expressing all three terms of (3.16) by (3.17), and eliminating $I_{m-1,q+2}$ by (3.14), we obtain

$$\begin{aligned}&\int_0^\infty\bigg(\alpha I_{m-1,q}(1, t)+I_{m-2,q-2}(1, t)-\sum_{b=1}^{m-1}\tilde{\Gamma}_b(q+2)\frac{t^{m-1-b}}{(m-1-b)!}-\alpha I_{m-1,q}(1, t)\\&\qquad+\alpha\sum_{b=1}^{m-1}\tilde{\Gamma}_b(q)\frac{t^{m-1-b}}{(m-1-b)!}-I_{m-2,q-2}(1, t)+\sum_{b=0}^{m-2}\tilde{\Gamma}_b(q-2)\frac{t^{m-2-b}}{(m-2-b)!}\bigg)\,\mathrm{d}t\\&=-\int_0^\infty\sum_{b=1}^{m-1}\frac{t^{m-1-b}}{(m-1-b)!}(\tilde{\Gamma}_b(q+2)-\alpha\tilde{\Gamma}_b(q)-\tilde{\Gamma}_{b-1}(q-2))\,\mathrm{d}t,\end{aligned}$$

which vanishes by the inductive hypothesis. Thus (3.16) is consistent with (3.17) at large q; $\tilde{\Gamma}_m(q)$ for small q is *defined* by solving (3.16) for its middle term and integrating. Next, we prove (3.18) for $q>2m$:

$$\begin{aligned}I_{m,q}(x, t)&=\int_0^t I_{m-1,q}(x, t')\,\mathrm{d}t'\\&=\int_0^t\sum_{b=1}^{m-1}\tilde{\Gamma}_b(q)x^{2b-q}\frac{(t')^{m-1-b}}{(m-1-b)!}\,\mathrm{d}t'\end{aligned}$$

$$+\int_0^t \left(I_{m-1,q}(x,t') - \sum_{b=1}^{m-1} \tilde{\Gamma}_b(q) x^{2b-q} \frac{(t')^{m-1-b}}{(m-1-b)!} \right) \mathrm{d}t'$$

$$= \sum_{b=1}^{m-1} \frac{\tilde{\Gamma}_b(q)}{(m-b)!} x^{2b-q} t^{m-b}$$

$$+\int_0^\infty \left(I_{m-1,q}(x,\tau x^2) - \sum_{b=1}^{m-1} \Gamma_b(q) x^{2m-2-q} \frac{\tau^{m-1-b}}{(m-1-b)!} \right) x^2 \, \mathrm{d}\tau$$

$$-\int_t^\infty (-1)^{m-1} (t')^{m-2-\alpha} \sum_{n=0}^\infty \frac{(-1)^n}{n!} \frac{\Gamma(\alpha+n+2-m)}{\Gamma(\alpha+n+1)} (x^2/t')^n \, \mathrm{d}t'$$

where (3.18) for $m-1$ guarantees convergence of the integrals at ∞ and has been used to re-express the integrand in the last term. According to lemma 2 and (3.17), the middle term equals $x^{2m-q}\tilde{\Gamma}_m(q)$. The last term can be integrated termwise, and the whole expression then reduces to (3.18). Finally, the series for $I_{m,q}$ with $q \leq 2m$ (but $q \neq 2, 0, -2, \ldots$) can be obtained from the cases already known, by solving (3.14) for $I_{m,q}$ and iterating as many times as required. A series obtained in this way must be consistent with (3.18) if q is actually still in the domain $q > 2m$; this guarantees the existence of a certain algebraic relation among the coefficients in the final term of (3.18) for adjacent values of q and m. Because Γ is meromorphic, this relation is valid for all q (away from the poles at $q = 2, 0, \ldots$); consequently, the series continues to have the form (3.18) when q is outside the original domain.

Comments. Part (ii) displays clearly the rapid decrease of every term in the heat expansion (3.7) as $t \to 0$ with $x \neq 0$ fixed; the terms in (3.10) come entirely from a region near the boundary, which shrinks as $t \to 0$. On the other hand, (3.10) cannot be obtained by inserting (3.18) into (3.7) and integrating finitely many terms; (3.18) carries terms of low order in κ and $V^{(n)}(0)$ arbitrarily far out into the series, accompanied by correspondingly large negative powers of t. Of course, (3.18) does yield an expansion of K_B in powers of the distance from the boundary which is valid for fixed $t \neq 0$. Lemma 2 can be interpreted as saying that $I_{m,q}(x,t)$ is a function only of the variable $y = x^2/t$, except for a trivial scaling factor. It follows that there is no expansion of K_B in elementary functions for x and t simultaneously small, since y ranges over the entire interval $0 < y < \infty$ inside any neighbourhood of the origin.

The $\mathrm{e}^{-x^2/t}$ behaviour of $K_\mathrm{B}(t,x,x)$ for large x or small t is reminiscent of the characteristic $\exp(-|x-y|^2/4t)$ behaviour of heat kernels, $K(t,x,y)$, at separated arguments. This should not come as a surprise. The Dirichlet and Neumann problems can be solved by the method of images (McKean and Singer 1967). In that approach, $K_\mathrm{B}(t,x,x)$ is found as $\pm K_0(t,x,-x)$, where K_0 is the heat kernel for a problem without boundary.

4. Piecewise smooth coefficients

The series derived in paper I for the spectral density, $\rho^{00}(\omega; x_0)$, and the corresponding series for the heat kernel, $K(t, x_0, x_0)$, contain coefficient functions involving increasingly high derivatives of $V(x_0)$. If some derivative of V fails to exist at x_0, all the terms of these series are undefined beyond a certain point—although ρ^{00} and K themselves are completely meaningful and finite at x_0. In fact, the series are not even trustworthy at other points x where V is smooth, because the derivation of the expansion of $\rho^{00}(\omega;x)$ assumes the *global* validity of the WKBF expansion (2.5) for the normalised eigenfunctions, but the WKBF expansion breaks down at x_0. (Actually, the heat-kernel expansion *is* valid at any point of smoothness, as is well known, but it will be seen that it is not valid uniformly in distance from the singularity at x_0.)

A moment's contemplation convinces one that a localised singularity ought to have spectral effects very similar to those of a boundary. (Indeed, in quantum mechanics it is traditional to regard a Dirichlet boundary as an infinite jump discontinuity in the potential (Messiah 1961, § III.4).) If the potential has compact support, one has a basis of scattering eigenfunctions with the behaviour indicated in (4.1) of I:

$$\phi_p(x) \sim \begin{cases} u_p\, \mathrm{e}^{\mathrm{i}px} + R_p\, \mathrm{e}^{-\mathrm{i}px} & \text{as } x \to -(\operatorname{sgn} p)\infty, \\ T_p\, \mathrm{e}^{\mathrm{i}px} & \text{as } x \to (\operatorname{sgn} p)\infty. \end{cases} \tag{4.1}$$

(Here u_p is a number of modulus one that can be chosen to simplify the relation between ϕ_p and the $\psi_{\lambda j}$.) However, because of the singularity, it is no longer true that, as stated in corollary 4.1 of I, $R_p = 0$ and $|T_p| = 1$ to all orders of the WKBF approximation. Instead, the reflected and transmitted waves will be of some finite order, determined by the nature of the singularity. The eigenfunctions for a boundary-value problem represent an extreme case where the reflected wave has intensity equal to that of the incident wave (see (2.10)). Since the boundary effects calculated earlier stem from the quantity $\operatorname{Re} \zeta_\omega(x)$ representing the interference between incident and reflected waves (see (2.18) and preceding calculation), it is clear that qualitatively similar effects will appear in the present situation.

For a certain class of singularities, detailed calculations can be done by an immediate extension of the methods employed previously in this series of papers. We make the following assumptions: $V(x)$ is a function of compact support on $\mathbb{R}$. $V(x)$ is infinitely differentiable except at $x=0$. The derivatives of order less than N exist at 0. The Nth derivative possesses finite, unequal right- and left-hand limits at 0, which we denote by $V^{(N)}(+0)$ and $V^{(N)}(-0)$. The higher derivatives also have finite limits from each side (possibly unequal).

The principal spectral density is given by (4.7) of I:

$$\rho^{00}(\omega;x) \equiv \pi\, \mathrm{d}\mu^{00}/\mathrm{d}\omega = \tfrac{1}{2}(|\phi_\omega(x)|^2 + |\phi_{-\omega}(x)|^2). \tag{4.2}$$

The ensuing calculation is parallel to those in § 4 of I and § 2 above. On each side of the singularity, express $\phi_{\pm\omega}(x)$ as a linear combination of WKBF basis functions, ψ_ω and $\psi_{-\omega}$. The eight coefficients can be determined, apart from some phases which do not enter (4.2), by imposing (4.1) and the conditions that $\phi_{\pm\omega}$ and $\phi'_{\pm\omega}$ are continuous at 0. Simplify the results by means of the easily verified identity

$$4Y_\omega(+0)Y_\omega(-0) + |N_\omega(-0) - N_\omega(+0)|^2 = |N_\omega(+0) + \overline{N_\omega(-0)}|^2. \tag{4.3}$$

Define $\rho_{\mathrm{J}}^{00}(\omega;x)$ to be the difference between $\rho^{00}(\omega;x)$ and the spectral density $(\sim Y_\omega(x)^{-1})$ for a smooth potential. One finds

$$\rho_{\mathrm{J}}^{00}(\omega;x) \sim \begin{cases} Y_\omega(x)^{-1} \operatorname{Re}\left[\dfrac{N_\omega(+0) - N_\omega(-0)}{\overline{N_\omega(+0)} + N_\omega(-0)} \exp\left(-2\mathrm{i}\omega \displaystyle\int_0^x Y(x')\,\mathrm{d}x'\right)\right] & \text{for } x>0 \\ Y_\omega(x)^{-1} \operatorname{Re}\left[\dfrac{N_\omega(-0) - N_\omega(+0)}{N_\omega(+0) + \overline{N_\omega(-0)}} \exp\left(-2\mathrm{i}\omega \displaystyle\int_0^x Y(x')\,\mathrm{d}x\right)\right] & \text{for } x<0. \end{cases} \tag{4.4}$$

This is the analogue of (2.18) for the problem at hand.

Recall that

$$N_\omega(x) = 1 + \sum_{n=2}^{\infty} \omega^{-n} N_n(x)$$

where the highest derivative occurring in N_n is $V^{(n-2)}$. Thus ρ_J^{00} is of order ω^{-N-2} under our assumptions. In particular, if $N = 0$, then

$$\frac{N_\omega(-0) - \overline{N_\omega(+0)}}{N_\omega(+0) + \overline{N_\omega(-0)}} = \tfrac{1}{4}(V(+0) - V(-0))\omega^{-2} + \mathrm{O}(\omega^{-3}). \tag{4.5}$$

Furthermore, $\rho_J^{00}(\omega)$ oscillates with an angular frequency equal in lowest order to $2|x|$ (the length of the classical path to the singularity and back). Clearly, one could calculate $K(t, x, x)$ as in § 3 and would obtain the characteristic factor $\mathrm{e}^{-x^2/t}$ once more. That is, for fixed t, the heat kernel contains a 'lump' spread over a neighbourhood of $x = 0$, which is completely missing from the usual local expansion of K. Of course, this term vanishes faster than any power of t as $t \to 0$ for fixed $x \neq 0$. Nevertheless it yields, via (3.9), a contribution of finite order in $t^{1/2}$ to the integral of K over a fixed interval around 0. (Note that all the terms in the expansion of the quantity in (4.5) will be well defined and finite, unlike the x integrals of the terms in the usual heat-kernel expansion, which would be infinite or ambiguous in the present case whenever they contain products of derivatives of V of order greater than N.)

In accordance with the general principle of the locally equivalent potential, one would expect these conclusions about the situation in the immediate neighbourhood of 0 to remain applicable when the potential has other singularities elsewhere, is not of compact support, etc. The spectral effects of these remote features, weakened by distance, will be superimposed—perhaps nonlinearly—on the dominant, locally determined phenomena. Perhaps the simplest example in which the joint effects of two singular features can be studied is an operator characterised by both a jump discontinuity and a boundary.

Let $V(x)$ be as before, except that this time the domain M terminates on the left at a Dirichlet endpoint: $\psi(-L) = 0$. A complicated calculation similar to the previous ones yields

$$\rho^{00}(\omega\,; x) \sim Y_\omega(x)^{-1}\Big(1 + \mathrm{Re}\,\zeta_\omega(x) + (4|B|^2 - 1) \times \Big\{1 - \mathrm{Re}\Big[\mathrm{e}^{-\mathrm{i}\omega W} \exp\Big(-2\mathrm{i}\omega \int_0^x Y(x')\,\mathrm{d}x'\Big)\Big]\Big\}\Big) \qquad \text{for } x < 0 \tag{4.6}$$

where

$$|B|^2 = Y(+0)Y(-0)|N(+0) + \overline{N(-0)} + (N(-0) - N(+0))\,\mathrm{e}^{\mathrm{i}\omega W}|^{-2} \tag{4.7}$$

$$\zeta_\omega(x) \equiv -\exp\Big(2\mathrm{i}\omega \int_{-L}^{x} Y_\omega(x')\,\mathrm{d}x'\Big) \tag{4.8}$$

$$W \equiv 2\int_{-L}^{0} Y_\omega(x')\,\mathrm{d}x'. \tag{4.9}$$

(The almost equally complicated, but less interesting, formula for the case $x > 0$ is omitted.) W can be interpreted as the action of the closed orbit of length $2L$ inside the 'potential well' $-L < x < 0$ (cf remark 2.1). $|B|$ is the modulus of the amplitude of the eigenfunction inside the well; the fact that it oscillates with frequency W has the quantum-mechanical interpretation that a sequence of 'resonances' exists with that spacing, due to the trapping of waves by reflection from the potential step (Messiah 1961, § III.6).

Obviously the first two terms in (4.6) are, respectively, the basic local spectral density for a smooth potential and the contribution of the boundary (cf (2.18) and (2.16)). Identifying ρ_J^{00} of (4.4) with a part of the remaining term is not so easy, however. Let us consider the case $N = 0$, so that the number multiplying $e^{i\omega W}$ in (4.7) is of order ω^{-2} (see 4.5)), and let us expand the denominator in (4.7) as a geometric series and work only to the lowest non-trivial order. After much algebraic reduction one obtains

$$\begin{aligned}\rho^{00}(\omega; x) - Y_\omega(x)^{-1}(1 + \operatorname{Re}\zeta_\omega(x))\\ &= \rho_J^{00}(\omega; x) - \tfrac{1}{2}(V(+0) - V(-0))\\ &\quad\times\left\{\operatorname{Re} e^{i\omega W} - \tfrac{1}{2}\operatorname{Re}\left[e^{2i\omega W}\exp\left(2i\omega\int_0^x Y(x')\,dx'\right)\right]\right\}\omega^{-2}\\ &\quad + O(\omega^{-3}) \qquad \text{for } x < 0.\end{aligned} \tag{4.10}$$

That is, all the terms in the remainder with frequencies independent of W go together to make up ρ_J^{00}, at least up to third order. (In fact, this has been verified by the author up to $O(\omega^{-6})$. Presumably it holds to all orders.) Those terms have frequency $\approx 2|x|$, and thus effectively dominate when $|x| \ll L$.

The remaining two terms in (4.10) have approximate frequencies $2L$ and $4L + 2x = 2L + 2(L - |x|)$, respectively. In the classical-path interpretation (remark 2.1), the first of these represents a path which returns to its starting point after reflecting off each end of the potential well, and the second corresponds to a particle that bounces off the boundary, the potential step, and then the boundary again, before returning to x. (The paths that reflect from only one end of the well have already been encountered in ρ_B and ρ_J.) Paths which hit the potential step more than once are met at higher order in ω^{-1}; for instance, the fourth-order terms include some corresponding to path lengths $2L + 2|x|$, $4L$ and $4L + 2(L - |x|)$. All these terms arising from the *combined* presence of the boundary and the discontinuity give rise to terms in the heat kernel which vanish rapidly as $t \to 0$, *uniformly* in x (at least as $e^{-L^2/t}$). They are, however, expected to make finite contributions, throughout the potential well, to the renormalised energy density of a quantum field (a generalised Casimir effect—see DeWitt (1975), Dowker and Critchley (1977), Balian and Duplantier (1977, 1978), etc).

A slight extension of the calculations of this section would give the spectral effects of a potential with a term proportional to the Dirac delta distribution. More general types of singularities, such as

$$V(x) \sim |x|^{-N} \qquad \text{as } x \to 0,$$

must give rise to similar effects, but quantitative investigation of them would require other techniques (namely, a WKBF expansion in the presence of coalescing turning points).

It is hoped that the analogy pointed out here between boundaries and coefficient singularities will be useful in approaching higher-dimensional problems in which the symbol of the operator has singularities localised on lower-dimensional submanifolds.

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