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Heat kernels for manifolds with boundary: applications to charged membranes

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Abstract. A formula for the energy corresponding to a potential ϕ obeying $(-\nabla^2 + \kappa^2)\phi = 0$ is derived as an expansion in κ^{-1} for manifolds with arbitrary smooth boundaries and either Neumann or Dirichlet boundary conditions. The first three terms in the expansion are explicitly determined and they agree with results of Duplantier in three dimensions for flat space. Careful attention in the Dirichlet case is given to ensuring a well defined regularized expression for the kernel on the boundary surface derived from the Green function so as to ensure an unambiguous finite expression for the energy.

Potential theory involving solutions of Laplace's or Poisson's equations and calculation of electrostatic energies in various configurations is one of the classical areas of applied mathematics. An interesting variation is obtained when the Laplacian $-\nabla^2$ is replaced by $-\nabla^2 + \kappa^2$ which is physically relevant to electrolytes in the linearized Debye–Hückel approximation with κ an inverse screening length. As discussed in more detail by Duplantier [1] it is of experimental interest to determine the electrostatic energy of electrolytes bounded by charged membranes of arbitrary shape. Theoretically Duplantier obtained the first few terms in an expansion in inverse powers of κ valid for $\kappa R \gg 1$ where R is a typical radius of curvature of the boundary.

In this paper we rederive these results and extend them to an arbitrary manifold $\mathcal{M}$ with coordinates x^μ, a metric $g_{\mu\nu}$ and dimension d, bounded by a smooth $(d-1)$-dimensional surface $\partial\mathcal{M}$ with coordinates $\hat{x}^i$ so that the boundary of $\mathcal{M}$ is specified by $x^\mu(\hat{x})$. The induced metric on ∂M is then $\hat{\gamma}_{ij}(\hat{x}) = g_{\mu\nu}(x)\partial x^\mu/\partial\hat{x}^i\, \partial x^\nu/\partial\hat{x}^j|_{x=x(\hat{x})}$.

For a surface charge density $\hat{\rho}(\hat{x})$ on $\partial\mathcal{M}$ the energy is expressed in terms of a potential $\phi(x)$ by

$$\mathcal{E} = \mathcal{E}_{\mathcal{M}} + \mathcal{E}_{\partial\mathcal{M}} \qquad \mathcal{E}_{\mathcal{M}} = \frac{1}{2}\int_{\mathcal{M}} \mathrm{d}v(\partial_\mu\phi\partial^\mu\phi + \kappa^2\phi^2) \qquad \mathcal{E}_{\partial\mathcal{M}} = \int_{\partial\mathcal{M}} \mathrm{d}S\,\hat{\rho}\phi \quad (1)$$

for $\mathrm{d}v = \mathrm{d}^d x\sqrt{g}$, $\mathrm{d}S = \mathrm{d}^{d-1}\hat{x}\sqrt{\hat{\gamma}}$. The two boundary conditions of particular interest are (i) $\phi(x(\hat{x})) = \hat{\varphi}(\hat{x})$ prescribed on $\partial\mathcal{M}$ with $\hat{\rho}$ determined by $\partial_n\phi(\hat{x}) \equiv n^\mu(\hat{x})\partial_\mu\phi(x)|_{x=x(\hat{x})} = \hat{\rho}(\hat{x})$ where $n^\mu(\hat{x})$ is the unit inward normal on $\partial\mathcal{M}$ and

(ii) $\hat{\rho}(\hat{\boldsymbol{x}})$ fixed on $\partial\mathcal{M}$ and so determining $\partial_n\phi = \hat{\rho}$. In either case the energy is minimized by requiring

$$\Delta\phi = 0 \qquad \Delta = -\nabla^2 + \kappa^2 \tag{2}$$

subject to the appropriate boundary conditions, which gives $\mathcal{E} = \frac{1}{2}\mathcal{E}_{\partial\mathcal{M}} = -\mathcal{E}_{\mathcal{M}}$. In case (i) the solution, by standard methods, is

$$\phi(x) = \int_{\partial\mathcal{M}} \mathrm{d}S'\, G_{\mathrm{D}}(x,x')\overleftarrow{\partial}'_n\big|_{x'=x(\hat{\boldsymbol{x}}')}\hat{\varphi}(\hat{\boldsymbol{x}}') \tag{3}$$

for $G_{\mathrm{D}}(x,x')$ the Dirichlet Green function satisfying $G_{\mathrm{D}}(x,x')\big|_{x=x(\hat{\boldsymbol{x}})} = 0$, while in case (ii)

$$\phi(x) = -\int_{\partial\mathcal{M}} \mathrm{d}S'\, G_{\mathrm{N}}(x,x')\big|_{x'=x(\hat{\boldsymbol{x}}')}\,\hat{\rho}(\hat{\boldsymbol{x}}') \tag{4}$$

for $G_{\mathrm{N}}(x,x')$ the Neumann Green function satisfying $\partial_n G_{\mathrm{N}}(x,x')\big|_{x=x(\hat{\boldsymbol{x}})} = 0$. In both cases $\Delta G_{\mathrm{D,N}}(x,x') = \delta^d(x,x')$. In case (i), at least formally,

$$\begin{aligned}\mathcal{E}_{\mathcal{M},\mathrm{D}} &= -\frac{1}{2}\int_{\partial\mathcal{M}} \mathrm{d}S\,\mathrm{d}S'\,\hat{\varphi}(\hat{\boldsymbol{x}})\,\mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')\,\hat{\varphi}(\hat{\boldsymbol{x}}')\\ \mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}') &= \partial_n G_{\mathrm{D}}(x,x')\overleftarrow{\partial}'_n\big|_{x=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')}\end{aligned} \tag{5}$$

and in case (ii)

$$\begin{aligned}\mathcal{E}_{\mathcal{M},\mathrm{N}} &= \frac{1}{2}\int_{\partial\mathcal{M}} \mathrm{d}S\,\mathrm{d}S'\,\hat{\rho}(\hat{\boldsymbol{x}})\,g(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')\,\hat{\rho}(\hat{\boldsymbol{x}}')\\ g(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}') &= G_{\mathrm{N}}(x,x')\big|_{x=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')}\end{aligned} \tag{6}$$

where $\mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')$ and $g(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')$ are symmetric kernels of $\partial\mathcal{M}$ defined in terms of the Green functions G_{D} and G_{N}.

To demonstrate an expansion of $\mathcal{E}_{\mathcal{M}}$ valid for large κ we use previously obtained results [2] on the asymptotic form of the heat kernel $\mathcal{G}_{\nabla^2}(x,x';\tau)$ corresponding to the operator $\mathrm{e}^{\tau\nabla^2}$ as $\tau\to 0$. This may be regarded as an extension of the well known DeWitt [3] asymptotic expansion, which gives information on the behaviour of $\mathcal{G}_{\nabla^2}$ as $\tau\to 0$ for x' in the neighbourhood of x, to the case of manifolds with a boundary. In general the heat kernel is related to the Green function for Δ as in (2) by

$$G(x,x') = \int_0^\infty \mathrm{d}\tau\,\mathrm{e}^{-\tau\kappa^2}\mathcal{G}_{\nabla^2}(x,x';\tau)\,. \tag{7}$$

In the Neumann case then from the definition (6)

$$g(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}') = \int_0^\infty \mathrm{d}\tau\,\mathrm{e}^{-\tau\kappa^2}\mathcal{G}_{\nabla^2,\mathrm{N}}(x,x';\tau)\big|_{x=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')} \tag{8}$$

for $\mathcal{G}_{\nabla^2,\mathrm{N}}$, the heat kernel defined for Neumann boundary conditions. In the Dirichlet case it is necessary to be more careful about the divergent behaviour for $\hat{x}' \to \hat{x}$ since the expression for $\mathcal{E}_{\mathcal{M},\mathrm{D}}$ in (5) has in general a non-integrable singularity at $\hat{x} = \hat{x}'$. Using results in the appendix we obtain the regulated definition

$$\mathcal{K}(\hat{x},\hat{x}') = \lim_{\epsilon\to 0}\bigg(\int_\epsilon^\infty \mathrm{d}\tau\,\mathrm{e}^{-\tau\kappa^2}\partial_n \mathcal{G}_{\nabla^2,\mathrm{D}}(x,x';\tau)\overleftarrow{\partial}'_n\big|_{x=x(\hat{x}),x'=x(\hat{x}')} - \frac{1}{(\pi\epsilon)^{1/2}}\,\delta_{\partial\mathcal{M}}(\hat{x},\hat{x}')\bigg) + \frac{1}{2}K(\hat{x})\,\delta_{\partial\mathcal{M}}(\hat{x},\hat{x}') \tag{9}$$

where $\delta_{\partial\mathcal{M}}(\hat{x},\hat{x}') = \delta^{d-1}(\hat{x}-\hat{x}')/\sqrt{\hat{\gamma}}$ is the delta function on $\partial\mathcal{M}$. The limit in (9) may be shown to exist in the sense of distributions or after integration over suitably smooth test functions on $\partial\mathcal{M}$. In the last term $K = \hat{\gamma}^{ij}K_{ij}$ where $K_{ij}(\hat{x})$ is the extrinsic curvature of $\partial\mathcal{M}$ which may be defined by $n_\mu(\partial^2 x^\mu/\partial\hat{x}^i\partial\hat{x}^j + \Gamma^\mu_{\sigma\rho}\partial x^\sigma/\partial\hat{x}^i\partial x^\rho/\partial\hat{x}^j) = K_{ij}$ for $\Gamma^\mu_{\sigma\rho}$ the Christoffel connection on $\mathcal{M}$.

For either Dirichlet or Neumann boundary conditions, or generalizations thereof, we have found a representation of $\mathcal{G}_{\nabla^2}$ in the neighbourhood of the boundary as a formal expansion in a parameter ϵ. If we define $\hat{\sigma}(\hat{x},\hat{x}')$ as the geodetic interval on $\partial\mathcal{M}$ satisfying $\hat{\gamma}^{ij}\partial_i\hat{\sigma}\partial_j\hat{\sigma} = 2\hat{\sigma}$ then assuming $\tau,\hat{\sigma} = \mathrm{O}(\epsilon^2)$ and with $\hat{\sigma}^i = \hat{\gamma}^{ij}\partial_j\hat{\sigma}$

$$\begin{aligned}\mathcal{G}_{\nabla^2,\mathrm{N}}(\tau)\big|_{\partial\mathcal{M}} = \frac{1}{(4\pi\tau)^{d/2}}\,\mathrm{e}^{-\hat{\sigma}/2\tau}\bigg[&2 + \frac{1}{2}\sqrt{\pi}\tau^{1/2}\Big(K + \frac{1}{2\tau}K_{ij}\hat{\sigma}^i\hat{\sigma}^j\Big)\\ &- \frac{1}{4}\sqrt{\pi}\tau^{1/2}\Big(\partial_i K\hat{\sigma}^i + \frac{1}{2\tau}\hat{\nabla}_k K_{ij}\hat{\sigma}^i\hat{\sigma}^j\hat{\sigma}^k\Big)\\ &+ \frac{1}{3}\tau(\hat{R} + 2R^0_{nn}) + \frac{1}{6}(\hat{R}_{ij} + R^0_{ninj})\hat{\sigma}^i\hat{\sigma}^j\\ &+ \frac{1}{15}\tau(K^2 + 7K^{ij}K_{ij}) + \frac{1}{30}(K_{ik}K^k{}_j + 3KK_{ij})\hat{\sigma}^i\hat{\sigma}^j\\ &+ \frac{7}{120}\frac{1}{\tau}K_{ij}K_{k\ell}\hat{\sigma}^i\hat{\sigma}^j\hat{\sigma}^k\hat{\sigma}^\ell + \mathrm{O}(\epsilon^3)\bigg]\,.\end{aligned} \tag{10}$$

$\hat{\nabla}_k$ is the covariant derivative acting on tensor fields on $\partial\mathcal{M}$ with $\hat{R}_{ij}$ the corresponding Ricci tensor, $\hat{R} = \hat{\gamma}^{ij}\hat{R}_{ij}$ the scalar curvature, and for $R_{\mu\nu\sigma\rho}$ the Riemann tensor on $\mathcal{M}$ $R^0_{ninj}(\hat{x}) = n^\mu(\hat{x})n^\nu(\hat{x})\partial x^\sigma/\partial\hat{x}^i\partial x^\rho/\partial\hat{x}^j R_{\mu\nu\sigma\rho}(x(\hat{x}))$, $R^0_{nn} = \hat{\gamma}^{ij}R^0_{ninj}$. Similarly in the Dirichlet case

$$\begin{aligned}\partial_n\mathcal{G}_{\nabla^2,\mathrm{D}}(\tau)\overleftarrow{\partial}'_n\big|_{\partial\mathcal{M}} = \frac{1}{(4\pi\tau)^{d/2}}\,\mathrm{e}^{-\hat{\sigma}/2\tau}\frac{1}{\tau}\bigg[&1 - \frac{1}{2}\sqrt{\pi}\tau^{1/2}\Big(K - \frac{1}{2\tau}K_{ij}\hat{\sigma}^i\hat{\sigma}^j\Big)\\ &+ \frac{1}{4}\sqrt{\pi}\tau^{1/2}\Big(\partial_i K\hat{\sigma}^i - \frac{1}{2\tau}\hat{\nabla}_k K_{ij}\hat{\sigma}^i\hat{\sigma}^j\hat{\sigma}^k\Big)\\ &+ \frac{1}{6}\tau\hat{R} + \frac{1}{12}\hat{R}_{ij}\hat{\sigma}^i\hat{\sigma}^j + \frac{1}{4}R^0_{ninj}\hat{\sigma}^i\hat{\sigma}^j\\ &+ \frac{1}{6}\tau(K^2 - K^{ij}K_{ij}) - \frac{1}{12}(K_{ik}K^k{}_j + 5KK_{ij})\hat{\sigma}^i\hat{\sigma}^j\\ &+ \frac{5}{48}\frac{1}{\tau}K_{ij}K_{k\ell}\hat{\sigma}^i\hat{\sigma}^j\hat{\sigma}^k\hat{\sigma}^\ell + \mathrm{O}(\epsilon^3)\bigg]\,.\end{aligned} \tag{11}$$

In order to apply these formulae in (8) and (9) to obtain an expansion in $1/\kappa$ we use the result

$$\frac{1}{(4\pi\tau)^{(d-1)/2}}\mathrm{e}^{-\hat{\sigma}/2\tau} \sim \delta_{\partial\mathcal{M}} + \tau\left(\hat{\nabla}^2 - \frac{1}{3}\hat{R}\right)\delta_{\partial\mathcal{M}} + \frac{1}{2}\tau^2\hat{\nabla}^2\hat{\nabla}^2\delta_{\partial\mathcal{M}} + \cdots. \tag{12}$$

Applying (10) and (12) in (8), since $\tau = \mathrm{O}(\kappa^{-2})$ and using $\hat{\nabla}_i\hat{\sigma}^j = \delta_i^j + \mathrm{O}(\epsilon^2)$, gives

$$g \sim \frac{1}{\kappa}\left[1 + \frac{1}{2\kappa}K + \frac{1}{4\kappa^2}\left(R^0_{nn} + K^{ij}K_{ij} + \frac{1}{2}K^2\right)\right]\delta_{\partial\mathcal{M}} + \frac{1}{2\kappa^3}\hat{\nabla}^2\delta_{\partial\mathcal{M}} + \mathrm{O}(\kappa^{-4}) \tag{13}$$

and likewise from (9) and (11)

$$\mathcal{K} \sim -\kappa\left[1 - \frac{1}{2\kappa}K - \frac{1}{4\kappa^2}\left(R^0_{nn} + K^{ij}K_{ij} - \frac{1}{2}K^2\right)\right]\delta_{\partial\mathcal{M}} + \frac{1}{2\kappa}\hat{\nabla}^2\delta_{\partial\mathcal{M}} + \mathrm{O}(\kappa^{-2}). \tag{14}$$

The leading term in the expansion for $\mathcal{K}$ is obtained by using

$$\lim_{\epsilon\to 0}\left(\int_\epsilon^\infty \mathrm{d}\tau\,\frac{1}{(4\pi\tau)^{1/2}}\,\frac{1}{\tau}\,\mathrm{e}^{-\kappa^2\tau} - \frac{1}{(\pi\epsilon)^{1/2}}\right) = -\kappa$$

where the negative sign of this $\mathrm{O}(\kappa)$ term in (14) is essential since on insertion in (5) it is required to give $\mathcal{E}_{\mathcal{M},\mathrm{D}} > 0$. The term proportional to K in (14), which is $\mathrm{O}(1)$ as $\kappa \to \infty$, originates solely from the last term on the right-hand side of (9) since the corresponding terms in (11) involving K are just of the form $K - K_{ij}\hat{\sigma}^i\hat{\sigma}^j/2\tau$ and on using (12) the resulting contribution vanishes. This is necessary as otherwise in (9) the potentially divergent integral $\int_\epsilon^\infty \mathrm{d}\tau\,\mathrm{e}^{-\kappa^2\tau}/\tau$ would be present.

Using (9) and (11) it is easy to calculate the leading singular terms in the short-distance limit, $\hat{\sigma} \to 0$, for the kernel $\mathcal{K}(\hat{x},\hat{x}')$

$$\mathcal{K} \sim \frac{\Gamma(\frac{1}{2}d)}{\pi^{d/2}}(2\hat{\sigma})^{-d/2} - \frac{\Gamma(\frac{1}{2}d - \frac{1}{2})}{4\pi^{d/2-1/2}}(2\hat{\sigma})^{1/2-d/2}\left(K - (d-1)\frac{K_{ij}\hat{\sigma}^i\hat{\sigma}^j}{2\hat{\sigma}}\right) \tag{15}$$

excluding the $\delta_{\partial\mathcal{M}}$ contribution. The two contributions shown in (15), proportional to $(2\hat{\sigma})^{-d/2}$ and $(2\hat{\sigma})^{-d/2+1/2}$, represent non-integrable singularities on $\partial\mathcal{M}$, although integrals with suitable test functions may be well defined regarding $\mathcal{K}$ as a distribution [4].

For practical applications of these results, as considered by Duplantier [1], $d = 3$ and the space $\mathcal{M}$ may be taken as flat so that $R^0_{nn} = 0$. In this case $\hat{R} = K^2 - K^{ij}K_{ij}$ and the eigenvalues of K_{ij} are $1/R_1$, $1/R_2$ are the principal radii of curvature of the boundary, and hence $K = 2/R = 1/R_1 + 1/R_2$ and $\hat{R} = 2/R_1R_2$. From (13) and (14)

$$\mathcal{E}_{\mathcal{M},\mathrm{N}} \sim \frac{1}{2\kappa}\int_{\partial\mathcal{M}}\mathrm{d}S\left[\hat{\rho}^2\left(1 + \frac{1}{\kappa R} + \frac{3}{2}\frac{1}{\kappa^2R^2} - \frac{1}{2}\frac{1}{\kappa^2R_1R_2}\right) - \frac{1}{2\kappa^2}\,\partial_i\hat{\rho}\partial^i\hat{\rho}\right] \tag{16a}$$

$$\mathcal{E}_{\mathcal{M},\mathrm{D}} \sim \frac{\kappa}{2}\int_{\partial\mathcal{M}}\mathrm{d}S\left[\hat{\varphi}^2\left(1 - \frac{1}{\kappa R} - \frac{1}{2}\frac{1}{\kappa^2R^2} + \frac{1}{2}\frac{1}{\kappa^2R_1R_2}\right) + \frac{1}{2\kappa^2}\,\partial_i\hat{\varphi}\partial^i\hat{\varphi}\right] \tag{16b}$$

which are in exact accord with the results of Duplantier [1], obtained by a very different method. For a two-dimensional boundary $\int_{\partial\mathcal{M}}\mathrm{d}S\,\hat{R} = 8\pi(1-g)$ where g is the genus of $\partial\mathcal{M}$, $g = 0$ for a sphere, so this is a purely topological term.

Appendix

In order to justify the presence of the delta-function term in $\mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')$, as calculated in (9), it is necessary to pay special attention to the singularities present at coincident points in the Green function $G(x,x')$ when integrating by parts if one point x lies on the boundary. Introducing an arbitrary smooth function $f(x)$ on $\mathcal{M}$, and on $\partial\mathcal{M}$ defining $\hat{f}(\hat{\boldsymbol{x}}) = f(x(\hat{\boldsymbol{x}}))$, then formally Green's theorem

$$\int_{\mathcal{M}} \mathrm{d}v' \left[\partial_n G_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}})} \nabla'^2 f(x') - \partial_n G_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}})} \overleftarrow{\nabla}'^2 f(x')\right]$$
$$= \int_{\partial\mathcal{M}} \mathrm{d}S'\, \mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')\hat{f}(\hat{\boldsymbol{x}}') - \int_{\partial\mathcal{M}} \mathrm{d}S'\, \partial_n G_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')} \partial_n f(\hat{\boldsymbol{x}}') \tag{17}$$

defines $\mathcal{K}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')$ and also $\partial_n G_{\mathrm{D}}(\hat{x},x')$ as linear maps, or distributions, on test functions on $\partial\mathcal{M}$, assuming that in (17) we set $\partial_n G_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}})}(\overleftarrow{\nabla}'^2 - \kappa^2) = 0$. For simplicity here we take $\kappa = 0$ without loss of generality.

To analyse potentially singular contributions in (17) we introduce a regularized Green function by modifying (7)

$$\begin{aligned} G^{\epsilon}_{\mathrm{D}}(x,x') &= \int_{\epsilon}^{\infty} \mathrm{d}\tau\, \mathcal{G}_{\nabla^2,\mathrm{D}}(x,x';\tau) \\ \mathcal{K}^{\epsilon}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}') &= \partial_n G^{\epsilon}_{\mathrm{D}}(x,x')\overleftarrow{\partial}'_n\big|_{x=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')} . \end{aligned} \tag{18}$$

After using the heat kernel equation, $\partial_\tau \mathcal{G}_{\nabla^2}(\hat{x},x';\tau) + \mathcal{G}_{\nabla^2}(\hat{x},x';\tau)\overleftarrow{\nabla}'^2 = 0$, and also by virtue of the Dirichlet boundary conditions satisfied by the regularized Green function, $\partial_n G^{\epsilon}_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}}),x'=x(\hat{\boldsymbol{x}}')} = 0$, we may write instead of (17)

$$\int_{\mathcal{M}} \mathrm{d}v'\, \partial_n G^{\epsilon}_{\mathrm{D}}(\hat{x},x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}})} \nabla'^2 f(x')$$
$$= \int_{\partial\mathcal{M}} \mathrm{d}S'\, \mathcal{K}^{\epsilon}(\hat{\boldsymbol{x}},\hat{\boldsymbol{x}}')\hat{f}(\hat{\boldsymbol{x}}') - \int_{\mathcal{M}} \mathrm{d}v'\, \partial_n \mathcal{G}_{\nabla^2,\mathrm{D}}(\hat{x},x';\epsilon)\big|_{\hat{x}=x(\hat{\boldsymbol{x}})} f(x') . \tag{19}$$

The left-hand side of (19) may be straightforwardly shown to have a smooth limit as $\epsilon \to 0$. On the right-hand side we employ our previously derived asymptotic expansion of the heat kernel $\mathcal{G}_{\nabla^2,\mathrm{D}}(x,x';\tau)$ based on using the natural coordinate system $x^\mu = (\boldsymbol{x},y)$ in the neighbourhood of $\partial\mathcal{M}$ where the metric takes the form

$$\mathrm{d}s^2 = \mathrm{d}y^2 + \gamma_{ij}(\boldsymbol{x},y)\mathrm{d}x^i\mathrm{d}x^j \qquad \gamma_{ij}(\boldsymbol{x},0) = \hat{\gamma}_{ij}(\boldsymbol{x}) .$$

With $\hat{x} = x(\hat{\boldsymbol{x}})$ $x' = (\boldsymbol{x}',y')$ and for $\hat{\sigma}(\hat{\boldsymbol{x}},\boldsymbol{x}') \sim \tau \to 0$ the asymptotic expansion leads to the expression relevant in (19)

$$\begin{aligned} &\partial_n \mathcal{G}_{\nabla^2,\mathrm{D}}(\hat{x},x';\tau) \\ &\quad\sim \frac{1}{(4\pi\tau)^{1/2d}}\, \mathrm{e}^{-\hat{\sigma}/2\tau}\, \frac{y'}{\tau}\bigg[\mathrm{e}^{-y'^2/4\tau}\left(1 + \frac{y'}{4\tau} K_{ij}\hat{\sigma}^i\hat{\sigma}^j\right) \\ &\qquad - \frac{1}{2}\int_{y'}^{\infty} \mathrm{d}z\, \mathrm{e}^{-z^2/4\tau}\left(K - \frac{1}{2\tau} K_{ij}\hat{\sigma}^i\hat{\sigma}^j\right)\bigg] \\ &\quad\sim \left(\frac{1}{(\pi\tau)^{1/2}} + \frac{1}{2}K\right)\delta(y')\delta_{\partial\mathcal{M}}(\boldsymbol{x},\boldsymbol{x}') \end{aligned} \tag{20}$$

using (12) and also

$$\theta(y')\mathrm{e}^{-y'^2/4\tau} \sim (\pi\tau)^{1/2}\delta(y') - 2\tau\delta'(y') + \sqrt{\pi}\tau^{3/2}\delta''(y') .$$

Hence in the limit $\epsilon \to 0$, using $\mathrm{d}v' \sim \mathrm{d}S'\mathrm{d}y'(1-y'K)$ and $f(x') \sim \hat{f}(\hat{\boldsymbol{x}}') + y'\partial_n f(\hat{\boldsymbol{x}}')$, then (19) becomes

$$\begin{aligned}\int_{\mathcal{M}} \mathrm{d}v'\, \partial_n G_{\mathrm{D}}(\hat{x}, x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}})} \nabla'^2 f(x') \\ = \lim_{\epsilon\to 0}\left(\int_{\partial\mathcal{M}} \mathrm{d}S'\, \mathcal{K}^{\epsilon}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')\hat{f}(\hat{\boldsymbol{x}}') - \frac{1}{(\pi\epsilon)^{1/2}}\hat{f}(\hat{\boldsymbol{x}})\right) \\ + \frac{1}{2}K(\hat{\boldsymbol{x}})\hat{f}(\hat{\boldsymbol{x}}) - \partial_n f(\hat{\boldsymbol{x}}) .\end{aligned} \tag{21}$$

Following (17) this is then in accord with (9) and also with the additional relation

$$\partial_n G_{\mathrm{D}}(\hat{x}, x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}}), x'=x(\hat{\boldsymbol{x}}')} = \delta_{\partial\mathcal{M}}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}') . \tag{22}$$

An alternative method of defining a regularized kernel is to follow textbook [5] procedures by excluding from $\mathcal{M}$ a region bounded by a hemisphere $\mathcal{S}_c$ so that for $x' \in \mathcal{S}_c$, x' is at a geodesic distance c from $\hat{x} = x(\hat{\boldsymbol{x}})$. For $x' \in \mathcal{S}_c$ assuming

$$\partial_n G_{\mathrm{D}}(\hat{x}, x') \qquad \partial_n G_{\mathrm{D}}(\hat{x}, x')\overleftarrow{\nabla}'^2 = \mathrm{O}(c^{-(d-1)}) \tag{23}$$

as $c \to 0$ the effect of the exclusion on the volume integration on the left-hand side of (17) vanishes in this limit. On the right-hand side of (17) $\int_{\partial\mathcal{M}} \to \int_{\partial\mathcal{M}_c} + \int_{\mathcal{S}_c}$ where for $x' \in \partial\mathcal{M}_c$ $\partial_n G_{\mathrm{D}}(\hat{x}, x') = 0$, by virtue of the Dirichlet boundary conditions satisfied by G_{D}, and further, $\mathcal{K}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')$ is defined by (5). In consequence it remains to determine the limiting form as $c \to 0$ of the integral

$$I_c = \int_{\mathcal{S}_c} \mathrm{d}S'\, \partial_n G_{\mathrm{D}}(\hat{x}, x')\overleftarrow{\partial}'_n f(x') - \int_{\mathcal{S}_c} \mathrm{d}S'\, \partial_n G_{\mathrm{D}}(\hat{x}, x')\, \partial_n f(x') . \tag{24}$$

To proceed further we employ our results on the asymptotic expansion of the heat kernel to obtain an explicit form for the leading singular terms in $\partial_n G_{\mathrm{D}}(\hat{x}, x')$.

If $\sigma(x, x')$ denotes the geodetic interval on $\mathcal{M}$, as calculated with the metric $g^{\mu\nu}$, which satisfies $\partial^\mu\sigma\partial_\mu\sigma = 2\sigma$, then for $x = \hat{x} = x(\hat{\boldsymbol{x}})$ it may be expanded as

$$\sigma(\hat{x}, x') = \tfrac{1}{2}y'^2 + \tfrac{1}{2}\hat{\gamma}_{ij}(\hat{\boldsymbol{x}})\hat{\sigma}^i\hat{\sigma}^j - \tfrac{1}{2}y'K_{ij}\hat{\sigma}^i\hat{\sigma}^j + \cdots$$

for $\hat{\sigma}^i(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')$. From its definition if $x' \in \mathcal{S}_c$, $2\sigma(\hat{x}, x') = c^2$ and letting $\xi_n(\hat{\boldsymbol{x}}, x') = -\partial_n\sigma(\hat{x}, x') = y' + \frac{1}{2}K_{ij}\hat{\sigma}^i\hat{\sigma}^j + \cdots$, $\xi_i(\hat{\boldsymbol{x}}, x') = -\partial_i\sigma(\hat{x}, x') = -\hat{\sigma}_i + \cdots$, then on $\mathcal{S}_c$, $\xi_n^2 + \hat{\gamma}^{ij}(\hat{\boldsymbol{x}})\xi_i\xi_j = c^2$. In terms of these variables we may write the required short-distance expansion, which is obtained from (20) and may be used to verify (23), as

$$\begin{aligned}\partial_n G_{\mathrm{D}}(\hat{x}, x') = \frac{\Gamma(\frac{1}{2}d)}{\pi^{d/2}}\,\xi_n(2\sigma)^{-d/2} - \frac{\Gamma(\frac{1}{2}d)}{2\pi^{d/2}}(2\sigma)^{-d/2+1}\frac{K_{ij}\hat{\sigma}^i\hat{\sigma}^j}{2\hat{\sigma}} \\ - y'\frac{\Gamma(\frac{1}{2}d-1)}{2\pi^{d/2}}\int_{y'}^{\infty}\mathrm{d}z\,\left(z^2 + 2\hat{\sigma}\right)^{-d/2+1}\left(K - (d-1)\frac{K_{ij}\hat{\sigma}^i\hat{\sigma}^j}{2\hat{\sigma}}\right) .\end{aligned} \tag{25}$$

On $\mathcal{S}_c$ $n_\mu = \partial'_\mu \sigma / c$ and since $\mathrm{d}v' = \sqrt{\hat{\gamma}}\,\mathrm{d}^d\xi[1 + \mathrm{O}(c^2)]$ we may write, using ξ_n, ξ_i to set up a Cartesian coordinate system with origin at $\hat{x} = x(\hat{\boldsymbol{x}})$

$$\mathrm{d}S' = c^{d-1}\mathrm{d}\Omega_d[1 + \mathrm{O}(c^2)] \qquad \int \mathrm{d}\Omega_d = S_d \equiv \frac{2\pi^{d/2}}{\Gamma(\frac{1}{2}d)}$$

with $\mathrm{d}\Omega_d$ the usual d-dimensional solid-angle element. If

$$\xi_n = c\cos\theta \qquad \mathrm{d}\Omega_d = S_{d-1}(\sin\theta)^{d-1}\mathrm{d}\theta\mathrm{d}\Omega_{d-1} \tag{26}$$

then the hemisphere $\mathcal{S}_c$ is defined by $0 < \theta < \frac{1}{2}\pi$. Writing (25) in terms of ξ_n, ξ_i and using $\partial'_n\sigma = 2\sigma/c$, $\partial'_n\xi_n = \xi_n/c$, $\partial'_n\xi_i = \xi_i/c$ on $\mathcal{S}_c$ we may then obtain

$$\begin{aligned}
\partial_n G_{\mathrm{D}}(\hat{x}, x')\overleftarrow{\partial}'_n &= -(d-1)\frac{\Gamma(\frac{1}{2}d)}{\pi^{d/2}}\frac{1}{c^d}\cos\theta + (d-2)\frac{\Gamma(\frac{1}{2}d)}{2\pi^{d/2}}\frac{1}{c^{d-1}}\frac{K_{ij}\xi^i\xi^j}{\xi^2} + \cdots \\
f(x') &= \hat{f}(\hat{\boldsymbol{x}}) + \xi_n\partial_n f(\hat{\boldsymbol{x}}) + \xi^i\partial_i\hat{f}(\hat{\boldsymbol{x}}) + \cdots \\
\partial'_n f(x') &= [\xi_n\partial_n f(\hat{\boldsymbol{x}}) + \xi^i\partial_i\hat{f}(\hat{\boldsymbol{x}})]/c + \cdots
\end{aligned} \tag{27}$$

neglecting terms which are ultimately negligible in I_c as $c \to 0$. Since, averaging over directions perpendicular to n^μ, $(d-1)\int \mathrm{d}\Omega_d\, K_{ij}\xi^i\xi^j = \int \mathrm{d}\Omega_d\, K\xi^2$, then from (27)

$$\begin{aligned}
I_c &\sim -\frac{1}{c}(d-1)\frac{\Gamma(\frac{1}{2}d)}{\pi^{d/2}}\hat{f}(\hat{\boldsymbol{x}})\int \mathrm{d}\Omega_d\,\cos\theta - d\frac{\Gamma(\frac{1}{2}d)}{\pi^{d/2}}\partial_n f(\hat{\boldsymbol{x}})\int \mathrm{d}\Omega_d\,\cos^2\theta \\
&\qquad + \frac{d-2}{d-1}\frac{\Gamma(\frac{1}{2}d)}{2\pi^{d/2}}K(\hat{\boldsymbol{x}})\hat{f}(\hat{\boldsymbol{x}})\int \mathrm{d}\Omega_d \\
&= -\frac{2}{c}\frac{S_{d-1}}{S_d}\hat{f}(\hat{\boldsymbol{x}}) - \partial_n f(\hat{\boldsymbol{x}}) + \frac{d-2}{2(d-1)}K(\hat{\boldsymbol{x}})\hat{f}(\hat{\boldsymbol{x}}).
\end{aligned} \tag{28}$$

Comparing this with (17) requires the result (22) again and also in this case

$$\begin{aligned}
\int_{\partial\mathcal{M}} \mathrm{d}S'\,\mathcal{K}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')\hat{f}(\hat{\boldsymbol{x}}') &= \lim_{c\to 0}\left(\int_{\partial\mathcal{M}, 2\hat{\sigma} > c^2} \mathrm{d}S'\,\mathcal{K}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')\hat{f}(\hat{\boldsymbol{x}}') - \frac{2}{c}\frac{S_{d-1}}{S_d}\hat{f}(\hat{\boldsymbol{x}})\right) \\
&\qquad + \frac{d-2}{2(d-1)}K(\hat{\boldsymbol{x}})\hat{f}(\hat{\boldsymbol{x}})
\end{aligned} \tag{29}$$

which ensures that $\mathcal{K}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')$ is a well defined kernel on $\partial\mathcal{M}$. Although (29) and (9), for $\kappa \to 0$, are rather different we have checked that the two prescriptions for defining $\mathcal{K}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')$ are equivalent. With the prescription (29) and re-introducing κ then the $\mathrm{O}(1)$ part as $\kappa \to \infty$ arises both from the regularized integral defined by the limit $c \to 0$ as well as the last term in (29), unlike the corresponding case for (9). For the specific example of $\mathcal{M}$ with a flat metric bounded by a sphere, when the Dirichlet Green function can be determined exactly for $\kappa = 0$, we have checked that the prescription (29) is just such as to give $\mathcal{E}_{\mathcal{M},\mathrm{D}} = 0$ for the boundary value $\hat{\varphi}$ a constant since trivially in this case $\phi = \hat{\varphi}$ throughout $\mathcal{M}$.

In the Neumann case the kernel $g(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}')$ does not have non-integrable singularities but corresponding calculations in this case show that for compatibility with (17) when $G_{\mathrm{D}} \to G_{\mathrm{N}}$ requires

$$\partial_n G_{\mathrm{N}}(\hat{x}, x')\big|_{\hat{x}=x(\hat{\boldsymbol{x}}), x'=x(\hat{\boldsymbol{x}}')} = -\delta_{\partial\mathcal{M}}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}}'). \tag{30}$$

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Note added in proof. For additional recent articles on this subject, see [6].

References

[1] Duplantier B 1990 Exact curvature energies of charged membranes of arbitrary shape *Physica* **168A** 179
[2] McAvity D M and Osborn H 1991 A Dewitt expansion of the heat kernel for manifolds with a boundary *Class. Quant. Grav.* **8** 603 (erratum 1992 **9** 317)
[3] DeWitt B S 1965 *Dynamical Theory of Groups and Fields* (London: Gordon and Breach)
[4] Gel'fand I M and Shilov G E 1964 *Generalised Functions* vol 1 (New York: Academic)
[5] Courant R and Hilbert D 1962 *Methods of Mathematical Physics* vol 2 (New York: Wiley)
[6] Duplantier B, Goldstein R E, Romero-Rochin V and Pesci A 1990 *Phys. Rev. Lett.* **65** 508
Goldstein R E, Pesci A and Romero-Rochin V 1990 *Phys. Rev.* A **41** 5504
Goldstein R E, Halsey T C and Leibig M 1991 *Phys. Rev. Lett.* **66** 1551
Duplantier B 1991 *Phys. Rev. Lett.* **66** 1555