On multi-particle Brownian survivals and the spherical Laplacian

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Abstract

The probability density function for survivals, that is for transitions without hitting a barrier, for a collection of particles driven by correlated Brownian motions is analyzed. The analysis is known to lead to a study of the spectrum of the Laplacian on domains on the sphere in higher dimensions. The first eigenvalue of the Laplacian governs the large time behavior of the probability density function and the asymptotics of the hitting time distribution. It is found that the solution leads naturally to a spectral function, a 'generating function' for the eigenvalues and multiplicities of the Laplacian. Analytical properties of the spectral function suggest a simple scaling procedure for determining the eigenvalues, readily applicable for a homogeneous collection of correlated particles. Comparison of the first eigenvalue with the available theoretical and numerical results for some specific domains shows remarkable agreement.

The case of a particle obeying Brownian motion on the real line under different boundary conditions have been well studied. For instance, in the simplest case of a single barrier, the probability density function for transition without hitting the barrier is expressible in closed form. No closed form solutions exist in the case of a collection of such particles driven by correlated Brownian motions. The problem of n particles each restricted by a barrier can be recast into that of solving the heat equation or the diffusion equation in a conical region in n dimensions. Within such a context, the problem has been addressed by various authors in the past and series solutions have been obtained. The $n = 2$ solution was obtained by Sommerfeld [1894]. It has been addressed within the context of default correlation by Zhou [2001]. The $n = 3$ case was considered within the context of circular cones by Carslaw and Jaeger [1959]. For higher dimensions, the applicable solution has been presented by Cheeger [1983]. The probability of survival as such was obtained by DeBlassie [1987] and its implications for hitting times discussed.

The radial component of the diffusion equation is identifiable with the differential equation for a Bessel process whose solution is well-known. The angular component of the series solution governing n Brownian particles involves the eigenvalues and the eigenfunctions of the Laplacian on a domain on the $n-1$ dimensional sphere. The first eigenvalue of the Laplacian determines the large time behavior of the survival probability and hence the finiteness of the expected hitting time. It is found that the solution leads naturally to a spectral function, a 'generating function' for the eigenvalues and their multiplicities, expressible in closed form for certain domains on the sphere such as the octant triangle on the

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two-sphere and analogous ones on higher dimensional spheres. Analytical properties of the spectral function suggest a simple scaling procedure to estimate the first few eigenvalues for related domains, readily applicable to the case of a homogeneous collection of correlated particles. The estimates for some specific domains are found to be in excellent agreement with the available theoretical and numerical results.

The article is organized as follows. Sections 1, 2 and 3 address the solutions for one, two and many particle systems. Section 4 discusses a spectral function for the Laplacian arising from the series solution. Section 5 analyzes some of the analytical properties of the spectral function. Section 6 discusses a scaling procedure to estimate the eigenvalues and their applicability to a homogeneous collection of correlated particles. Section 7 compares the estimates with some of the available theoretical and numerical results. An extension of the scaling procedure is presented in the appendix.

1 One Particle

Consider a particle driven by Brownian motion on the real line with position variable x. The probability density $f(x, x', \tau)$ that the particle at position x at any time t reaches x' at time $t + \tau$ is obtained by solving the differential equation

$$\frac{\partial f}{\partial \tau} = \frac{1}{2}\frac{\partial^2 f}{\partial x^2}. \tag{1}$$

A constant drift term may be present but is ignored for simplicity. A scaling of x is done to standardize the coefficient of the second order term. The above is the well-studied heat equation or the diffusion equation in one dimension having the fundamental solution

$$f(x, x', \tau) = \frac{1}{\sqrt{2\pi\tau}} e^{-\frac{1}{2\tau}(x-x')^2}. \tag{2}$$

As required, $f(x, x', \tau) \to \delta(x - x')$ as $\tau \to 0$.

Consider next a barrier at $x = 0$. We will now be interested in the probability density that the particle at $x > 0$ at any time t reaches $x' > 0$ at time $t + \tau$ without hitting the barrier. The requirement that the particle does not hit the barrier can be stated as Dirichlet boundary condition $f(0, x', \tau) = 0$ corresponding to a perfectly absorbing boundary. The solution to the differential equation is easily obtained by the method of images,

$$f(x, x', \tau) = \frac{1}{\sqrt{2\pi\tau}}\left(e^{-\frac{1}{2\tau}(x-x')^2} - e^{-\frac{1}{2\tau}(x+x')^2}\right) = \sqrt{\frac{2}{\pi\tau}} e^{-\frac{1}{2\tau}(x^2+x'^2)} \sinh\left(\frac{xx'}{\tau}\right). \tag{3}$$

The total probability $p(x, \tau)$ that the particle travels without hitting the barrier, the probability of surviving absorption at the boundary, is then

$$p(x, \tau) = \int_0^\infty dx' f(x, x', \tau) = 1 - 2N\left(-\frac{x}{\sqrt{\tau}}\right), \tag{4}$$

where N is the cumulative standard normal distribution function. This has the large-time behavior $\sim \tau^{-\frac{1}{2}}$ resulting in an infinite expected hitting time.

Though our concern in the article is with Dirichlet boundary conditions, we may note here that under Neumann boundary condition $\frac{\partial f}{\partial x}(0, x', \tau) = 0$ corresponding to a perfectly reflecting boundary, one would have cosh in place of sinh in (3). We may also note that a constant drift at rate μ would result in an additional term $\mu\frac{\partial f}{\partial x}$ on the right hand side of (1) whose effect is to multiply the Dirichlet solution (3) with $e^{-\mu(x-x')-\frac{1}{2}\mu^2\tau}$.

2 Two Particles

Next consider two particles on the real line with positions x_1 and x_2, together denoted $\boldsymbol{x}$, driven by Brownian motions correlated with a correlation parameter ρ. Let the barriers be at zero, that is at $x_1 = 0$ for the first particle and $x_2 = 0$ for the second. The domain we are concerned with for $\boldsymbol{x}$ is hence the first quadrant in the (x_1, x_2) plane. The transition probability density $\frac{1}{\sqrt{1-\rho^2}} f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ that the particles at $\boldsymbol{x} > 0$, that is $x_1 > 0$ and $x_2 > 0$, at any time t reach $\boldsymbol{x}' > 0$ at time $t + \tau$ without either of them hitting the barrier is now governed by the differential equation

$$\frac{\partial f}{\partial \tau} = \frac{1}{2} \left[\frac{\partial^2 f}{\partial x_1^2} + 2\rho \frac{\partial^2 f}{\partial x_1 \partial x_2} + \frac{\partial^2 f}{\partial x_2^2} \right], \tag{5}$$

subject to Dirichlet boundary conditions $f(\boldsymbol{x}, \boldsymbol{x}', \tau)\,|_{x_1=0} = f(\boldsymbol{x}, \boldsymbol{x}', \tau)\,|_{x_2=0} = 0$. As before, for simplicity, constant drift terms are ignored and a suitable scaling of x_1 and x_2 is done to standardize the coefficients. The above equation can be diagonalized with change of coordinates, for instance with

$$y_1 = \frac{1}{\sqrt{1-\rho^2}} (x_1 - \rho x_2), \quad y_2 = x_2. \tag{6}$$

In the new system of coordinates, the differential equation becomes

$$\frac{\partial f}{\partial \tau} = \frac{1}{2} \left[\frac{\partial^2 f}{\partial y_1^2} + \frac{\partial^2 f}{\partial y_2^2} \right]. \tag{7}$$

This is the heat equation or the diffusion equation in two dimensions. The boundaries $x_1 = 0, x_2 > 0$ and $x_2 = 0, x_1 > 0$ in the new coordinate system read

$$y_1 = -\frac{\rho}{\sqrt{1-\rho^2}} y_2, \quad y_2 > 0 \quad \text{and} \quad y_2 = 0, \quad y_1 > 0. \tag{8}$$

It is convenient to go to polar coordinates r and θ where

$$r = \sqrt{y_1^2 + y_2^2}, \quad \theta = \cos^{-1}\left(\frac{y_1}{r}\right), \quad 0 \le \theta \le \varphi = \cos^{-1}(-\rho). \tag{9}$$

The boundaries are now at $\theta = 0$ and $\theta = \varphi$. The differential equation to be solved reads

$$\frac{\partial f}{\partial \tau} = \frac{1}{2} \left[\frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} \right]. \tag{10}$$

Angular functions $\sin(\nu\theta)$ can be chosen to vanish on the boundaries so that $f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ can be expanded in Fourier series as

$$f(\boldsymbol{x}, \boldsymbol{x}', \tau) = \sum_\nu g_\nu(r, \boldsymbol{x}', \tau) r^\nu \sin(\nu\theta), \quad \nu = \frac{k\pi}{\varphi}, \quad k = 1, 2, \cdots. \tag{11}$$

The differential equation now reduces to

$$\frac{\partial g_\nu}{\partial \tau} = \frac{1}{2}\frac{\partial^2 g_\nu}{\partial r^2} + \frac{2\nu + 1}{2r}\frac{\partial g_\nu}{\partial r}. \tag{12}$$

This is the differential equation describing the Bessel process. Its solution is well-known: $\frac{r'^2}{\tau}$ is distributed as the non-central chi-squared distribution with $2(\nu+1)$ degrees of freedom and non-centrality parameter $\frac{r^2}{\tau}$. We thus have for the r'-distribution

$$g_\nu\left(r, \boldsymbol{x}', \tau\right) \sim \frac{2r'}{\tau}\chi^2\left(\frac{r'^2}{\tau}, 2(\nu+1), \frac{r^2}{\tau}\right) = \frac{r'}{\tau}\left(\frac{r}{r'}\right)^{-\nu} e^{-\frac{1}{2\tau}\left(r^2+r'^2\right)} I_\nu\left(\frac{rr'}{\tau}\right), \tag{13}$$

where I_ν is the modified Bessel function. Putting together, we have

$$f(\boldsymbol{x}, \boldsymbol{x}', \tau) = \frac{2}{\varphi\tau} e^{-\frac{1}{2\tau}\left(r^2+r'^2\right)} \sum_\nu I_\nu\left(\frac{rr'}{\tau}\right) \sin(\nu\theta)\sin(\nu\theta'). \tag{14}$$

To verify the factors, note that $dx_1 dx_2 = \sqrt{1-\rho^2} r dr d\theta$, and that $f(\boldsymbol{x}, \boldsymbol{x}', t) \to \frac{1}{r'}\delta(r - r')\delta(\theta-\theta') = \sqrt{1-\rho^2}\delta(x_1 - x_1')\delta(x_2 - x_2')$ in the limit $\tau \to 0$. The asymptotic behavior $I_\nu(x) \to (2\pi x)^{-\frac{1}{2}} e^x, x \to \infty$ for fixed ν gives rise to $\delta(r-r')$ in the form of a limiting normal distribution in $\frac{1}{\sqrt{\tau}}(r-r')$ (roughly, since the series involves sum over $\nu \to \infty$).

The above result was obtained differently by Sommerfeld [1894]. It has been addressed within the context of default correlation by Zhou [2001]. The total probability of survival $p(\boldsymbol{x}, \tau)$ can be obtained by integrating over r' and θ',

$$p(\boldsymbol{x}, \tau) = \sqrt{\frac{2\pi}{\tau}} \frac{r}{\varphi} e^{-\frac{r^2}{4\tau}} \sum_{\nu \text{ odd}} \frac{1}{\nu}\left[I_{\frac{\nu+1}{2}}\left(\frac{r^2}{4\tau}\right) + I_{\frac{\nu-1}{2}}\left(\frac{r^2}{4\tau}\right)\right] \sin(\nu\theta), \tag{15}$$

where by ν odd, it is meant that the integers k in (11) are restricted to be odd.

3 Many Particles

We now come to a collection of n particles on the real line with positions $x_i, i = 1, 2, \cdots, n$, together denoted by a position vector $\boldsymbol{x}$, driven by Brownian motions correlated with a correlation matrix R. The barriers are set at zero, that is at $x_i = 0$ for the i^{th} particle, so that the domain D^n we are concerned with for $\boldsymbol{x}$ is $x_i > 0, i = 1, \cdots, n$. The transition probability density $\frac{1}{\sqrt{\det R}} f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ that the particles at $\boldsymbol{x}$ within the domain at any time t reach $\boldsymbol{x}'$ within the domain at time $t+\tau$ without any of them hitting the barrier is now governed by the differential equation

$$\frac{\partial f}{\partial \tau} = \frac{1}{2}\sum_{ij} R_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j}, \tag{16}$$

subject to Dirichlet boundary conditions on the boundary of D^n: $f(\boldsymbol{x}, \boldsymbol{x}', \tau)\,|_{x_i=0} = 0$ (that is, when any one of the x_i's is set to zero). It is also expected that $f(\boldsymbol{x}, \boldsymbol{x}', \tau) \to 0$ when any one of the x_i's is taken to infinity. Generally one would have a covariance matrix on the right hand side above. For convenience, x_i's are suitably scaled so that the covariance matrix is replaced by the correlation matrix. Constant drift terms may also be present but are ignored for simplicity.

As before, it is convenient to work in the diagonalized system that diagonalizes R and scales it into identity so that the differential equation involves the Laplacian ∇^2,

$$\frac{\partial f}{\partial \tau} = \frac{1}{2}\nabla^2 f, \quad \nabla^2 = \sum_i \frac{\partial^2}{\partial y_i^2}. \tag{17}$$

This is the heat equation or the diffusion equation in n dimensions. Dot-products defined as $\boldsymbol{u} \cdot \boldsymbol{v} = \sum_{ij} R^{-1}_{ij} u_i v_j$ for any two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ and the implied lengths remain invariant but now get diagonalized expressions. It is further convenient to split the coordinates $\boldsymbol{y}$ into radial and angular parts, r and $\hat{\boldsymbol{r}}$,

$$r^2 = \sum_i y_i^2 = \sum_{ij} R^{-1}_{ij} x_i x_j, \quad \hat{\boldsymbol{r}} = \frac{\boldsymbol{y}}{r}. \tag{18}$$

In the diagonalized system, domain D^n remains conical intersecting into a domain Ω^{n-1} traced out by the unit radial vectors $\hat{\boldsymbol{r}}$ on the $n-1$ dimensional sphere S^{n-1} at $r^2 = 1$. Dirichlet boundary conditions require $f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ to vanish on the boundary $\partial\Omega^{n-1}$. If desired, Neumann boundary conditions can be defined in the diagonalized system as usual with the normal derivatives required to vanish on the boundary.

Functions on Ω^{n-1} can be equivalently expressed as zero-degree (positive-)homogeneous functions in D^n. Solving the Laplace equation $\nabla^2(r^\nu h_{\nu\sigma}) = 0$ in D^n for a ν-degree homogeneous function $r^\nu h_{\nu\sigma}(\hat{\boldsymbol{r}})$ is equivalent to solving the Laplacian eigenvalue problem[1]

$$\nabla^2_S h_{\nu\sigma}(\hat{\boldsymbol{r}}) = -\lambda h_{\nu\sigma}(\hat{\boldsymbol{r}}), \quad \lambda = \nu(\nu + n - 2) \tag{19}$$

for a zero-degree homogeneous function $h_{\nu\sigma}(\hat{\boldsymbol{r}})$. Here $\nabla^2_S = r^2\nabla^2$ acting on functions of $\hat{\boldsymbol{r}}$ is the Laplacian on S^{n-1} and hence on Ω^{n-1}, and $h_{\nu\sigma}(\hat{\boldsymbol{r}})$ is the eigenfunction vanishing on $\partial\Omega^{n-1}$, σ labeling any multiplicity. Boundary value problems of the above kind have been extensively studied and it turns out that the eigenvalues are all real, non-negative and discrete, and that the eigenfunctions can be taken to be real and form a complete system. Hence ν's can also be taken to be real, non-negative and discrete and we will assume that the eigenfunctions are normalized to form an orthonormal system

$$\int_{\Omega^{n-1}} d^{n-1}\hat{r} h_{\nu\sigma}(\hat{\boldsymbol{r}}) h_{\nu'\sigma'}(\hat{\boldsymbol{r}}) = \delta_{\nu\nu'}\delta_{\sigma\sigma'}, \tag{20}$$

where $d^{n-1}\hat{r}$ is the volume element on the unit sphere S^{n-1} (area element if S^2).

The complete system of eigenfunctions $h_{\nu\sigma}(\hat{\boldsymbol{r}})$ enables us to expand $f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ as

$$f(\boldsymbol{x}, \boldsymbol{x}', \tau) = \sum_{\nu\sigma} g_{\nu\sigma}(r, \boldsymbol{x}', \tau) r^\nu h_{\nu\sigma}(\hat{\boldsymbol{r}}). \tag{21}$$

The Laplacian on $g_{\nu\sigma} r^\nu h_{\nu\sigma}$ separates into that on $g_{\nu\sigma} r^\nu$ and $h_{\nu\sigma}$. Its action on $h_{\nu\sigma}$ is given by (19) so that the differential equation for $f(\boldsymbol{x}, \boldsymbol{x}', \tau)$ gives rise to

$$\frac{\partial g_{\nu\sigma}}{\partial \tau} = \frac{1}{2}\frac{\partial^2 g_{\nu\sigma}}{\partial r^2} + \frac{2\nu + n - 1}{2r}\frac{\partial g_{\nu\sigma}}{\partial r}. \tag{22}$$

This is again the differential equation describing the Bessel process. Hence, $\frac{r'^2}{\tau}$ is distributed as the non-central chi-squared distribution with $2\nu + n$ degrees of freedom and non-centrality parameter $\frac{r^2}{\tau}$. We thus have for the r'-distribution,

$$g_{\nu\sigma}\left(r, \boldsymbol{x}', \tau\right) \sim \frac{2r'}{\tau}\chi^2\left(\frac{r'^2}{\tau}, 2\nu + n, \frac{r^2}{\tau}\right) = \frac{r'}{\tau} e^{-\frac{1}{2\tau}\left(r^2 + r'^2\right)} \left(\frac{r}{r'}\right)^{-\nu - \frac{n-2}{2}} I_{\nu + \frac{n-2}{2}}\left(\frac{rr'}{\tau}\right), \tag{23}$$

[1] ∇^2 acting on a product $g(r)h(\hat{\boldsymbol{r}})$ separates into $(\nabla^2 g)h + g(\nabla^2 h)$ when $h(\hat{\boldsymbol{r}})$ is zero-degree homogeneous function because of the vanishing of the cross term $(\nabla g) \cdot (\nabla h) = \partial_r(g) r^{-1}(\boldsymbol{y} \cdot \nabla)h = 0$.

where again I_ν is the modified Bessel function. Putting these together, we have

$$f(\boldsymbol{x},\boldsymbol{x}',\tau)=\frac{1}{\tau}(rr')^{-\frac{n-2}{2}}e^{-\frac{1}{2\tau}(r^2+r'^2)}\sum_\nu I_{\nu+\frac{n-2}{2}}\left(\frac{rr'}{\tau}\right)\sum_\sigma h_{\nu\sigma}(\hat{\boldsymbol{r}})h_{\nu\sigma}(\hat{\boldsymbol{r}}'). \tag{24}$$

To verify the factors, note that the integration measure is $d^nx=\sqrt{\det R}r^{n-1}drd^{n-1}\hat{r}$, and that $f(\boldsymbol{x},\boldsymbol{x}',\tau)\to\sqrt{\det R}\delta(\boldsymbol{x}-\boldsymbol{x}')$ in the limit $\tau\to 0$. The asymptotic behavior $I_\nu(x)\to(2\pi x)^{-\frac{1}{2}}e^x, x\to\infty$ for fixed ν gives rise to $\delta(r-r')$ in the form of a limiting normal distribution in $\frac{1}{\sqrt{\tau}}(r-r')$ (roughly, since the series involves sum over $\nu\to\infty$). The presence of a constant drift at rate $\boldsymbol{\mu}$ would result in an additional term $\sum_i \mu_i\frac{\partial f}{\partial x_i}$ on the right hand side of (16) whose effect is to multiply $f(\boldsymbol{x},\boldsymbol{x}',\tau)$ with $e^{-\boldsymbol{\mu}\cdot(\boldsymbol{x}-\boldsymbol{x}')-\frac{1}{2}\boldsymbol{\mu}^2\tau}$.

The above result was obtained differently under different contexts by various authors. For $n=2$ it was obtained by Sommerfeld [1894]. For $n=3$, it was considered within the context of circular cones by Carslaw and Jaeger [1959]. For general dimensions, it has been presented by Cheeger [1983]. The leading term in the series (24) can be obtained by making use of the expansion for the Bessel functions,

$$f(\boldsymbol{x},\boldsymbol{x}',\tau)\sim\frac{2}{\Gamma\left(\nu_1+\frac{n}{2}\right)(2\tau)^{\frac{n}{2}}}\left(\frac{rr'}{2\tau}\right)^{\nu_1}e^{-\frac{1}{2\tau}(r^2+r'^2)}h_{\nu_1}(\hat{\boldsymbol{r}})h_{\nu_1}(\hat{\boldsymbol{r}}'), \tag{25}$$

where ν_1 is the first ν and Γ is the Gamma function. In the case of an independent collection of particles in the presence of barrier, we know that $f(\boldsymbol{x},\boldsymbol{x}',\tau)$ is given by the product of individual expressions (3) so that

$$f(\boldsymbol{x},\boldsymbol{x}',\tau)=\left(\frac{2}{\pi\tau}\right)^{\frac{n}{2}}e^{-\frac{1}{2\tau}(r^2+r'^2)}\prod_{i=1}^n\sinh\left(\frac{x_ix_i'}{\tau}\right). \tag{26}$$

In this case, series (24) provides an expansion of product of sinh's in terms of modified Bessel functions.

The total probability of survival $p(\boldsymbol{x},\tau)$ can be obtained by integrating $f(\boldsymbol{x},\boldsymbol{x}',\tau)$ with respect to $\boldsymbol{x}'$ on D^n giving (in the absence of drift)

$$p(\boldsymbol{x},\tau)=\tau^{\frac{n}{2}}r^{-n}e^{-\frac{r^2}{2\tau}}\sum_\nu\widetilde{I}_{\nu+\frac{n-2}{2}}\left(\frac{r^2}{\tau}\right)\sum_\sigma h_{\nu\sigma}(\hat{\boldsymbol{r}})\widetilde{h}_{\nu\sigma}, \tag{27}$$

where

$$\widetilde{I}_{\nu+\frac{n-2}{2}}(a)=\int_0^\infty dt\,t^{\frac{n}{2}}e^{-\frac{t^2}{2a}}I_{\nu+\frac{n-2}{2}}(t)\quad\text{and}\quad\widetilde{h}_{\nu\sigma}=\int_{\Omega^{n-1}}d^{n-1}\hat{r}h_{\nu\sigma}(\hat{\boldsymbol{r}}). \tag{28}$$

This result in terms of a hypergeometric function was obtained as the solution of a differential equation by DeBlassie [1987] who also discussed its implications for hitting times. The first term in the series is guaranteed to be positive since it is well known that the first $h_{\nu\sigma}$ can be taken to be positive within the domain. For large τ, $p(\boldsymbol{x},\tau)$ has the behavior $\sim\tau^{-\frac{\nu_1}{2}}$, implying that the expected hitting time will be finite if $\nu_1>2$. As discussed in the next section, for an independent collection of particles, $\nu_1=n$ so that the expected hitting time will be finite for $n\geq 3$. For a positively correlated collection of particles we expect $\nu_1<n$ but greater than $n-1$ as long as correlations are not too large so that the expected hitting time will remain finite for $n\geq 3$.

4 Spectrum On The Sphere

The solution for the transition probability density obtained in the last section is expressed in terms of the eigenvalues and the eigenfunctions of the Laplacian on the sphere. Hence, let us have a look into the spectrum of the Laplacian on a domain Ω^{n-1} on the sphere S^{n-1} in n-dimensions corresponding to a collection of n particles.

Domain Ω^{n-1} for n independent particles in the presence of barrier, denoted as Ω_0^{n-1}, occupies $(2^{-n})^{\text{th}}$ of S^{n-1} obtained by cutting away the sphere into half, n-times. For instance, Ω_0^1 is given by the quadrant circular arc. Ω_0^2 is given by the octant triangle on the two-sphere, a triangular region having three $90°$ angles. It can be viewed as an extension of Ω_0^1 into the third dimension. Ω_0^{n-1} in higher dimension can be similarly approached. For the correlated case in the presence of barrier, Ω^1 is a circular arc, Ω^2 is a spherical triangle, Ω^3 is a spherical tetrahedron and Ω^{n-1} in higher dimension is an analogous domain (a spherical polytope) on S^{n-1}. Ω^{n-1} has n boundary segments corresponding to n barriers, each of which is part of a great sphere S^{n-2} and is of type Ω^{n-2} with the elements of the correlation matrix R as the cosine of the angles between their normals.

Many results are known in general about the eigenvalues and eigenfunctions of the Laplacian for such domains. For instance, the first eigenvalue has no multiplicity and the corresponding eigenfunction can be taken to be positive within the domain. In the case of independent particles in the absence of barrier, the domain is the whole of S^{n-1} and the resulting spectrum is well-known. In this case ν is an integer taking values from zero to infinity. The first ν, denoted ν_1, is zero corresponding to a constant function on S^{n-1}. The multiplicities of the eigenvalues will be revisited below.

In the independent case in the presence of barrier, it is straightforward to show that $\nu_1 = n$. In fact, being independent, the simplest homogeneous function solving the Laplace equation in D^n and vanishing on the boundaries is of degree n and is given simply by the product of the n-coordinates consistent with equation (26). It is further clear that adding an independent particle with barrier to a correlated collection would increase ν_1 by one. If the added independent particle is not subject to the boundary condition, ν_1 would remain the same. These observations are not trivial when formulated on the sphere.

To say more about the spectrum of the Laplacian on the sphere, let us next derive a spectral function, a 'generating function' for the eigenvalues and multiplicities in terms of $f(\boldsymbol{x}, \boldsymbol{x}', \tau)$. Towards this end, let us set $\boldsymbol{x}' = \boldsymbol{x}$ and $\tau = 1$ to obtain

$$f(\boldsymbol{x}, \boldsymbol{x}, 1) = r^{2-n} e^{-r^2} \sum_{\nu} I_{\nu + \frac{n-2}{2}} \left(r^2\right) \sum_{\sigma} (h_{\nu\sigma}(\hat{\boldsymbol{r}}))^2. \tag{29}$$

Note that a further operation of integrating over $\boldsymbol{y}$, along with any $\hat{r}$-independent weight, would integrate $(h_{\nu\sigma}(\hat{\boldsymbol{r}}))^2$ to unity (its normalization) introducing the multiplicity m_ν. This procedure derives the following expression for the spectral function $M(z)$ making use of the Laplace transform of I_ν,

$$M(z) \equiv \sum_{\nu} m_\nu z^\nu = \left(1 - z^2\right) z^{-\frac{n}{2}} \int_{D^n} d^n y \, e^{-\frac{1}{2z}(1-z)^2 r^2} f(\boldsymbol{x}, \boldsymbol{x}, 1), \tag{30}$$

where $0 < z < 1$ and r is the length of $\boldsymbol{x}$ or $\boldsymbol{y}$ as given by (18). If the right side can be computed, this would provide us with both the eigenvalues and the multiplicities.

The above function arose naturally from the solution of the heat equation on the cone. It differs from the usually studied trace of the heat kernel, $\mathrm{Tr} e^{t\nabla_S^2}$, in that it is not the eigenvalues $\nu(\nu+n-2)$ of $-\nabla_S^2$ that appear in the exponents, but rather ν's themselves. Its derivation did not assume any specific character of the domain, except that D^n is conical intersecting S^{n-1} into some domain Ω^{n-1}. But its applicability depends on our knowledge of $f(\boldsymbol{x},\boldsymbol{x},1)$. This is not expected to be the case in general. Below, let us first consider some special cases for which we do know $f(\boldsymbol{x},\boldsymbol{x},1)$.

Consider again the case of independent particles with no barrier. In this case the integration range covers all of $\boldsymbol{x}$, that is, it includes $\boldsymbol{x}<0$ as well. Knowing $f(\boldsymbol{x},\boldsymbol{x},1) = (2\pi)^{-\frac{n}{2}}$ as a product from n-individual free Brownian motions at $\boldsymbol{x}=\boldsymbol{x}', \tau=1$ (see (2)), one readily obtains

$$M(z) = (1-z^2)(1-z)^{-n} = 1 + nz + \sum_{k=2}^{\infty}\left[\binom{n+k-1}{k} - \binom{n+k-3}{k-2}\right] z^k. \tag{31}$$

This gives the right eigenvalues and multiplicities on the whole sphere S^{n-1}. The two terms inside square brackets are the dimensions of the spaces of degree k and degree $k-2$ homogeneous polynomials in n variables, and the role of $1-z^2$ is hence to choose the difference for the dimension of the space of degree k harmonic homogeneous polynomials, that is those satisfying the Laplace equation in n-dimensions.

In the case of independent particles with barrier, $f(\boldsymbol{x},\boldsymbol{x},1)$ is given by (26) that generates the spectral function

$$M(z) = z^n(1-z^2)^{1-n} = \sum_{k=1}^{\infty}\binom{n+k-3}{k-1} z^{n+2k-2}. \tag{32}$$

As noted earlier, this corresponds to a domain Ω_0^{n-1} on S^{n-1} that is 2^{-n} of its size obtained by cutting away the sphere into half, n-times: a quadrant arc on S^1, an octant triangle on S^2 or an analogous domain on a higher dimensional sphere. In the case of two correlated particles, we know from section 2 that ν's are multiples of $\frac{\pi}{\varphi}$ and are all of multiplicity one. Its spectral function is hence $z^{\frac{\pi}{\varphi}}(1-z^{\frac{\pi}{\varphi}})^{-1}$ that becomes $z^2(1-z^2)^{-1}$ in the independent case corresponding to a quadrant arc in agreement with (32). For Neumann boundary conditions, factor z^n in front above is absent.

Note that $M(z)$, except for the factor $1-z^2$, factorizes across subsystems that are mutually independent but may well be internally dependent. Hence, $M(z)$ for a system comprising of two subsystems independent of each other with spectral functions $M_1(z)$ and $M_2(z)$ that are not necessarily of the independent types is given by

$$M(z) = \frac{1}{1-z^2}M_1(z)M_2(z). \tag{33}$$

For example, if we have $n=p+q$ independent particles of which p particles have no barrier and q ones do, the product system has

$$M(z) = z^q(1-z)^{-p}(1-z^2)^{1-q}. \tag{34}$$

This corresponds to a domain on S^{n-1} that is obtained by cutting away the sphere into half, q-times. For instance, with $p=n-1, q=1$, this gives $M(z)=z(1-z)^{1-n}$ as the spectral function for the half-sphere. Knowing the spectral function for correlated pairs of particles, one or more of such pairs can also be included in the above expression.

If we are interested in exploring the $h_{\nu\sigma}(\hat{\boldsymbol{r}})$ functions themselves, we could rederive our results without the angular integration to obtain

$$M(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}',z)\equiv\sum_{\nu}m_{\nu}(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}')z^{\nu}=(1-z^{2})z^{-\frac{n}{2}}\int_{0}^{\infty}dr\,r^{n-1}e^{-\frac{1}{2z}(1-z)^{2}r^{2}}f(r\hat{\boldsymbol{x}},r\hat{\boldsymbol{x}}',1),\tag{35}$$

where $m_{\nu}(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}')=\sum_{\sigma}h_{\nu\sigma}(\hat{\boldsymbol{r}})h_{\nu\sigma}(\hat{\boldsymbol{r}}')$. This provides us with a spectral function for the projections on to the eigenspaces. As a function of $z\hat{\boldsymbol{r}}$ with z considered as a radial coordinate, it can be identified as a kernel satisfying the Laplace equation on the cone inside the unit sphere under Dirichlet boundary conditions tending to $\delta(\hat{\boldsymbol{r}}-\hat{\boldsymbol{r}}')$ as $z\to 1$. In the case of n independent particles without barrier, that is on the whole sphere S^{n-1}, we get

$$M(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}',z)=\frac{1}{|S^{n-1}|}\frac{1-z^{2}}{(1-2z\cos\theta+z^{2})^{\frac{n}{2}}},\qquad \left|S^{n-1}\right|=\frac{2\pi^{\frac{n}{2}}}{\Gamma\left(\frac{n}{2}\right)},\tag{36}$$

where θ is the angle between $\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{r}}'$, and $\left|S^{n-1}\right|$ is the size of the sphere S^{n-1} (surface area if S^2). This is the Poisson kernel of the n-dimensional unit ball at points $z\hat{\boldsymbol{r}}$ and $\hat{\boldsymbol{r}}'$ that when expanded in powers of z gives rise to zonal harmonics as projections in terms of Gegenbauer (ultraspherical) polynomials. Expressions involving more such terms can be obtained in other independent cases by setting one or more directions to have barrier.

One may also be interested in inverting (30) to obtain information about the heat kernel on the cone when the spectral function on a domain on the sphere is known. Given $M(z)$ on a domain Ω^{n-1}, one can obtain $f_{\Omega^{n-1}}(t)$, where $f_{\Omega^{n-1}}(r^2)=r^{n-2}\int_{\Omega^{n-1}}d^{n-1}\hat{r}\,f(\boldsymbol{x},\boldsymbol{x},1)$, as the Laplace inverse of $\widehat{f}_{\Omega^{n-1}}(s)=\frac{2z^{\frac{n}{2}}}{1-z^2}M(z), z=1+s-\sqrt{s(s+2)}$, or obtain its 'trace' $\int_0^r dr r f_{\Omega^{n-1}}(r^2)$ as the Laplace inverse of $\frac{1}{2s}\widehat{f}_{\Omega^{n-1}}(s)$. For instance, in the independent case with barrier, knowing $M(z)$ from (32), $f_{\Omega^{n-1}}(r^2)$ can be obtained as the Laplace inverse of $\frac{1}{2^{n-1}}\left(\frac{1+s-\sqrt{s(s+2)}}{s(s+2)}\right)^{\frac{n}{2}}$. The inverse is easily carried out for $n=2$ to give

$$\int_{\Omega_0^1}d\hat{r}\,f(\boldsymbol{x},\boldsymbol{x},1)=\frac{1}{4}-\frac{1}{2}I_0\left(r^2\right)e^{-r^2}+\frac{1}{4}e^{-2r^2}.\tag{37}$$

Here Ω_0^1 is the quadrant arc and I_0 is the modified Bessel function of order zero (this can also be obtained directly from the series solution (14); alternately, knowing $M(z)$, Laplace inverse can be viewed as summing up certain series of Bessel functions.). More generally, one can obtain $r^{n-2}f(r\hat{\boldsymbol{x}},r\hat{\boldsymbol{x}}',1)$ inverting (35) as the Laplace inverse of $\frac{2z^{\frac{n}{2}}}{1-z^2}M(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}',z)$.

5 Analytical Properties

On continuing from the $z<1$ region, $M(z)$ exhibits a singularity at $z=1$. At least for the various cases considered, the singularity is a pole of order $n-1$ (the dimension of the sphere) so that we may write around $z=1$

$$M(z)=\frac{c_0}{(1-z)^{n-1}}+\frac{c_1}{(1-z)^{n-2}}+\cdots.\tag{38}$$

Coefficients c_0 and c_1 can be determined,

$$c_0=2\frac{\left|\Omega^{n-1}\right|}{\left|S^{n-1}\right|},\quad c_1=-\frac{1}{2}c_0-\frac{1}{2}\frac{\left|\partial\Omega^{n-1}\right|}{\left|S^{n-2}\right|}.\tag{39}$$

It is convenient to write $c_1 = -\frac{1}{2}(1+\gamma)c_0$ introducing

$$\gamma = -2\frac{c_1}{c_0} - 1 = \frac{1}{2}\frac{\left|S^{n-1}\right|}{\left|S^{n-2}\right|}\frac{\left|\partial\Omega^{n-1}\right|}{\left|\Omega^{n-1}\right|}. \tag{40}$$

Here, $\left|S^{n-1}\right|$ and $\left|S^{n-2}\right|$ are the sizes of $n-1$ and $n-2$ dimensional spheres of unit radii respectively. $\left|\Omega^{n-1}\right|$ is the size of the domain Ω^{n-1} and $\left|\partial\Omega^{n-1}\right|$ is that of its boundary $\partial\Omega^{n-1}$. Sizes of Ω^{n-1} and $\partial\Omega^{n-1}$ are measured in units set by the $n-1$ dimensional sphere S^{n-1} of unit radius on which they reside. For Neumann boundary conditions, the expression for γ will have a negative sign.

The leading coefficient c_0 can be determined by letting $z \to 1$ in the expression for $M(z)$. Note that the exponential inside the integral would no longer provide the suppression as $r \to \infty$. As $r \to \infty$, $f(\boldsymbol{x}, \boldsymbol{x}, 1)$ away from the boundary tends to a constant $(2\pi)^{-\frac{n}{2}}$ (n factors from (2) at $\boldsymbol{x} = \boldsymbol{x}', \tau = 1$). The integral is thus dominated by regions near $r = \infty$ where the angular integral contributes $\left|\Omega^{n-1}\right|$. This gives, as $\epsilon = 1 - z \to 0$,

$$M(1-\epsilon) \sim 2\epsilon \int_0^\infty dr\, r^{n-1} e^{-\frac{1}{2}\epsilon^2 r^2} \frac{\left|\Omega^{n-1}\right|}{(2\pi)^{\frac{n}{2}}} = 2\frac{\Gamma\left(\frac{n}{2}\right)}{2\pi^{\frac{n}{2}}}\frac{\left|\Omega^{n-1}\right|}{\epsilon^{n-1}}. \tag{41}$$

The factors in front can be identified as twice the inverse size of the sphere S^{n-1}.

The next coefficient c_1 can be determined by the method of images. To start with, note that the contribution to $M(z)$ coming from the source alone,

$$\frac{c_0}{2}\frac{1+z}{(1-z)^{n-1}} = \frac{c_0}{(1-z)^{n-1}} - \frac{1}{2}\frac{c_0}{(1-z)^{n-2}}, \tag{42}$$

makes an order $n-1$ contribution as well. In the method of images, the source placed within the domain induces images across the boundary that cancel out the source effect on the boundary to ensure zero boundary condition. Since $f(\boldsymbol{x}, \boldsymbol{x}, 1)$ is evaluated at the source location itself, as $\boldsymbol{x}$ is varied, the source moves and the images follow the source. As $r \to \infty$ many of the images will recede away from the source. The leading contribution comes from the image brought closest to the source by taking the source close to the boundary. Its contribution is $\sim -(2\pi)^{-\frac{n}{2}} e^{-2y_\perp^2}$. Here $y_\perp$ is the perpendicular distance of the source to the boundary so that the image to source distance is $2y_\perp$. The image contribution as $\epsilon = 1 - z \to 0$ is

$$-\frac{2\epsilon}{(2\pi)^{\frac{n}{2}}} \int_0^\infty dr\, r^{n-2} e^{-\frac{1}{2}\epsilon^2 r^2} \int_{\partial\Omega\perp} dy_\perp\, e^{-2y_\perp^2} = -\frac{1}{2}\frac{\Gamma\left(\frac{n-1}{2}\right)}{2\pi^{\frac{n-1}{2}}}\frac{\left|\partial\Omega^{n-1}\right|}{\epsilon^{n-2}}. \tag{43}$$

The factors in front can be identified as half the inverse size of the sphere S^{n-2}. A negative sign is chosen to satisfy Dirichlet boundary conditions on the boundary. For Neumann boundary conditions, the sign will be positive.

Expansion (38) is a result of an expansion of $f(\boldsymbol{x}, \boldsymbol{x}, 1)$ in r^{-1} in the expression (30) for $M(z)$. Since $\tau^{\frac{n}{2}} f(\boldsymbol{x}, \boldsymbol{x}, \tau)$ is function of the combination $\frac{r^2}{\tau}$, an expansion of $f(\boldsymbol{x}, \boldsymbol{x}, 1)$ in r^{-1} is in fact an expansion of $f(\boldsymbol{x}, \boldsymbol{x}, \tau)$ in $\sqrt{\tau}$ at $\tau = 1$. This is the well-known expansion of the heat kernel (see for instance Vassilevich [2003]), in our case on the cone D^n. Because the higher order terms of this expansion bring in more powers of r into the denominator inside the integral in (30), as such it can only be used upto coefficient c_{n-1}. If the remainder falls off faster than r^{-n} as $r \to \infty$, its integral will be finite at $z = 1$ because of the $r \to 0$

behavior of $f(\boldsymbol{x},\boldsymbol{x},1)$ evident from (29). Also note here that the heat kernel expansion being an expansion in r^{-1} does not see any terms of the type e^{-r} for instance. That such terms are present can be seen by taking the example of the $n=2$ independent system with barrier for which we know $\int_{\Omega_0^1} d\hat{r}\, f(\boldsymbol{x},\boldsymbol{x},1)$ from (37). The first two terms on the right hand side of (37) give rise to the heat kernel expansion while the last term, not visible to the heat kernel asymptotics, is required for the $r\to 0$ behavior.

Expansion (38) can also be obtained from the heat kernel expansion on Ω^{n-1} on the sphere itself. This can be done using the identity

$$M\left(e^{-s}\right)=\frac{se^{\ell s}}{2\sqrt{\pi}}\int_0^\infty \frac{dt}{t^{\frac{3}{2}}}e^{-\ell^2 t-\frac{s^2}{4t}}\mathrm{Tr}e^{t\nabla_S^2}, \tag{44}$$

where Tr refers to trace and $\ell=\frac{1}{2}(n-2)$. Analogous relation can be written down for the pointwise object $M(\hat{\boldsymbol{r}},\hat{\boldsymbol{r}}',z)$. Inverse relations can be obtained by expressing them as Laplace transforms, giving rise to identities for the heat kernel such as the one involving the Jacobi θ-function on S^1.

The series expansion of the kind at the $z=1$ pole are useful in estimating the growth of the spectrum at large eigenvalues. This is done with the help of a counting function $W(\nu)=\sum_{\nu'} m_{\nu'}1_{\nu'\le\nu}$, where $1_{\nu'\le\nu}$ is the step-function, that counts the eigenvalues, including multiplicity, up to ν. Its Laplace transform is

$$\widetilde{W}(s)=\int_0^\infty d\nu W(\nu)e^{-s\nu}=\frac{1}{s}M(e^{-s}). \tag{45}$$

As we have noted, $M(e^{-s})$ is expected to have a pole of order $n-1$ at $s=0$. Here it should arise from the large ν behavior of $W(\nu)$. One finds

$$W(\nu)\sim\frac{c_0\nu^{n-1}}{(n-1)!}+\frac{1}{2}(n-2-\gamma)\frac{c_0\nu^{n-2}}{(n-2)!}+\cdots. \tag{46}$$

Expressed in terms of the eigenvalues $\lambda=\nu(\nu+n-2)\sim\nu^2$ of the Laplacian on Ω^{n-1}, this is consistent with the Weyl scaling law (true for more general domains).

As a Dirichlet series in s, one expects $M(e^{-s})$ defined on the positive real s-axis to be analytic on the half-plane $\mathrm{Re}(s)>0$. Its behavior for $\mathrm{Re}(s)\le 0$ is less clear. Result (30) indicates naively a relation $M\left(z^{-1}\right)=-z^{n-2}M(z)$. However, this is not expected to hold as an approach to z^{-1} from z along the real axis encounters the singularity at $z=1$. For the cases considered earlier, one finds instead $M\left(z^{-1}\right)=(-1)^{n-1}z^{n-2-\gamma}M(z)$ as well as $M_D\left(z^{-1}\right)=(-1)^{n-1}z^{n-2}M_N(z)$ where subscripts refer to Dirichlet and Neumann boundary conditions. Being consistent with the product formula (33), these will also hold for domains factorizable into such cases. They are however restrictive to hold in general, but when one does, $M(e^{-s})$ can be expected to be analytic on the half-plane $\mathrm{Re}(s)<0$ (with singularities along the imaginary s-axis).

6 A Scaling Procedure

It is a result that the eigenvalues of the Laplacian do not increase as the domain is enlarged. For a positively correlated collection of particles, domain Ω^{n-1} tends to be larger compared to Ω_0^{n-1} of the independent case, and hence we expect the eigenvalues to be nonincreasing with respect to overall correlation. Having dimensions of inverse coordinate squared, eigenvalues can be expected to scale accordingly, though in general approximately, suggesting that we look for a scaling procedure to estimate the eigenvalues in the correlated system. However, applying scaling to the eigenvalues itself, as is usually done, turns out to be not satisfactory. Let us hence look for a spectral function $M(z)$ on a target domain Ω^{n-1} of the form (for Dirichlet boundary conditions)

$$M(z) = z^{\alpha} M_0(z^{\beta}), \tag{47}$$

where $M_0(z)$ is the known spectral function on a reference domain Ω_0^{n-1}. This implies that, given the eigenvalues $\lambda_{0k} = \nu_{0k}(\nu_{0k} + n - 2), k = 1, 2, \cdots$ of the Laplacian on Ω_0^{n-1}, the eigenvalues $\lambda_k = \nu_k(\nu_k + n - 2)$ on Ω^{n-1} can be estimated according to

$$\nu_k = \alpha + \beta \nu_{0k}, \quad k = 1, 2, \cdots. \tag{48}$$

Parameters α and β can be determined by expanding $M(z)$ and $M_0(z)$ into their series (38) at $z = 1$ and matching the first two coefficients (39) for the two domains,

$$\alpha = \frac{1}{2}\left[\gamma - \beta\gamma_0 + (\beta - 1)(n-2)\right], \quad \beta = \left[\frac{\left|\Omega_0^{n-1}\right|}{\left|\Omega^{n-1}\right|}\right]^{\frac{1}{n-1}}, \tag{49}$$

where γ and γ_0 for Ω^{n-1} and Ω_0^{n-1} are as given by (40). This estimation procedure can also be expressed as a scaling of the combination $\nu + \frac{1}{2}(n - 2 - \gamma)$. Note that this does not change multiplicities. If Ω^{n-1} and Ω_0^{n-1} are closely related and the eigenvalues are well separated, this may be a reasonable assumption to make; at least for the first few eigenvalues. Eigenfunctions will of course be different.

The above procedure requires computing the domain sizes $\left|\Omega^{n-1}\right|$ and $\left|\partial\Omega^{n-1}\right|$. For a correlated system, $\left|\Omega^{n-1}\right|$ can be computed as

$$\left|\Omega^{n-1}\right| = \frac{\left|S^{n-1}\right|}{\sqrt{\det R}(2\pi)^{\frac{n}{2}}} \int_0^{\infty} d^n x \, e^{-\frac{1}{2}x^T R^{-1} x}, \tag{50}$$

while for the independent case it is given by $\left|\Omega_0^{n-1}\right| = 2^{-n}\left|S^{n-1}\right|$. $\left|\partial\Omega^{n-1}\right|$ can be computed using the same formula with R^{-1} restricted to one dimension less. An example of a correlated system is a homogeneous collection of particles with a single correlation parameter $\rho \geq 0$ such that the correlation matrix is

$$R_{ij} = (1-\rho)\delta_{ij} + \rho, \quad R_{ij}^{-1} = \frac{1}{1-\rho}\delta_{ij} - \frac{\rho}{(1-\rho)(1+(n-1)\rho)}. \tag{51}$$

This matrix has determinant $\det R = (1-\rho)^{n-1}(1+(n-1)\rho)$. Diagonalization to coordinates y_i can be carried out for instance by

$$x_i = a y_i + b\sum_{j=1}^{n} y_j, \quad y_i = \frac{1}{a}x_i - \frac{b}{a(a+nb)}\sum_{j=1}^{n} x_j,$$
$$a = \sqrt{1-\rho}, \quad b = \frac{1}{n}\left(\sqrt{1+(n-1)\rho} - \sqrt{1-\rho}\right). \tag{52}$$

As noted in section 3, in the diagonalized coordinate system, ρ can be identified as the cosine of the angle between the normals to boundary segments. For this homogeneous system, the domain size expression (50) simplifies to

$$\left|\Omega^{n-1}\right| = \left|S^{n-1}\right| \int_{-\infty}^{\infty} \frac{du}{\sqrt{2\pi}} e^{-\frac{1}{2}u^2}\left[N\left(\frac{\sqrt{\rho}\,u}{\sqrt{1-\rho}}\right)\right]^n, \tag{53}$$

where N is the cumulative standard normal distribution function. The same expression upon setting $n \to n-1$ and $\rho \to \frac{\rho}{1+\rho}$ gives $\frac{1}{n}\left|\partial\Omega^{n-1}\right|$. It can be evaluated for $\rho = \frac{1}{2}$ for any n giving $\left|\Omega^{n-1}\right| = \frac{1}{n+1}\left|S^{n-1}\right|$ corresponding to a domain on S^{n-1} analogous to a tetrahedral triangle on the two-sphere. For general ρ, $f_n(\rho) = \frac{\left|\Omega^{n-1}\right|}{\left|\Omega_0^{n-1}\right|}$ obeys the recursive differential equation

$$\frac{\partial}{\partial\rho} f_n(\rho) = \frac{n(n-1)}{\pi\sqrt{1-\rho^2}} f_{n-2}\left(\frac{\rho}{1+2\rho}\right), \tag{54}$$

with $f_0(\rho) = f_1(\rho) = f_n(0) = 1$. For $n = 2$, this gives $\left|\Omega^1\right| = \cos^{-1}(-\rho)$ in agreement with section 1 and for $n = 3$, it gives $\left|\Omega^2\right| = 3\cos^{-1}(-\rho) - \pi$ consistent with the identification of $\cos^{-1}(-\rho)$ as the vertex angle of the spherical equilateral triangle Ω^2 (having $\left|\partial\Omega^2\right| = 3\cos^{-1}\left(-\frac{\rho}{1+\rho}\right)$). For very small ρ, $f_n(\rho) \approx 1 + \frac{1}{\pi}n(n-1)\rho$ so that $\alpha \approx -\frac{1}{\pi}n(n-2)\rho$ and $\beta \approx 1 - \frac{1}{\pi}n\rho$ giving $\nu_1 \approx n - \frac{2}{\pi}n(n-1)\rho$. Since $f_n(\rho)$ is an increasing function of ρ, we have $\left|\Omega^{n-1}\right| > \left|\Omega_0^{n-1}\right|$. As $\rho \to 1$, $f_n(\rho) \to 2^{n-1}$ so that Ω^{n-1} tends to cover half the sphere. Since $M(z) = z(1-z)^{1-n}$ of the half-sphere is exactly related by scaling to $M_0(z) = z^n(1-z^2)^{1-n}$ of the $\rho = 0$ domain Ω_0^{n-1}, scaling estimates could be reasonable for ρ in-between. This is confirmed by a numerical comparison discussed below.

7 Numerical Comparisons

The following numerical comparisons are for domains on the two-sphere of unit radius. For clarity, area $\left|\Omega^2\right|$ is denoted as A and the perimeter $\left|\partial\Omega^2\right|$ as L so that for the scaling parameters (49), we have $\gamma = \frac{L}{A}, \gamma_0 = \frac{L_0}{A_0}, \beta = \sqrt{\frac{A_0}{A}}, \alpha = \frac{1}{2}[\gamma - 1 - \beta(\gamma_0 - 1)]$.

The domain on the two-sphere corresponding to a homogeneous collection of three correlated particles having correlation ρ is a spherical equilateral triangle of vertex angle $\cos^{-1}(-\rho)$. It has $A = 3\cos^{-1}(-\rho) - \pi$ and $L = 3\cos^{-1}\left(-\frac{\rho}{1+\rho}\right)$. In this case, the reference domain for scaling estimation can be chosen to be the octant triangle having $M_0(z) = z^3(1-z^2)^{-2}$, $A_0 = \frac{\pi}{2}, L_0 = \frac{3\pi}{2}, \gamma_0 = \nu_{01} = 3$. Ratzkin and Treibergs [2009] have studied a capture problem that can be recast into that of a homogeneous collection having $\rho = \frac{1}{2}$. For $\rho = \frac{1}{2}$, the spherical equilateral triangle is a tetrahedral triangle having $A = \pi, L = 3\cos^{-1}\left(-\frac{1}{3}\right)$. The authors present a theoretical and numerical result 5.159 for the first eigenvalue $\lambda_1 = \nu_1(\nu_1 + 1)$ of the Laplacian on the tetrahedral triangle. Scaling estimate gives $\nu_1 = 1.826$ and $\lambda_1 = 5.162$ in excellent agreement with their result, indicating that the scaling procedure should be satisfactory for homogeneous collections.

A spherical cap is a circular domain on the two-sphere. If its radius relative to its center in angles is θ, it has $A = 2\pi(1 - \cos\theta)$ and $L = 2\pi\sin\theta$. In this case the reference domain can be chosen to be the half-sphere that has $M_0(z) = z(1-z)^{-2}, \gamma_0 = \nu_{01} = 1$ so that

$$\nu_1 = \frac{1}{2}\left(\cot\frac{\theta}{2} - 1\right) + \frac{\nu_{01}}{\sqrt{2}\sin\frac{\theta}{2}}. \tag{55}$$

The usual scaling procedure applied to the eigenvalues of the Laplacian itself is based on just the size of the domain, and hence is not able to differentiate the effects of the boundary. Ratzkin and Treibergs [2009] present a theoretical result $\lambda_1 = 4.936$ for the first eigenvalue on a spherical cap ($\theta = \frac{\pi}{3}$) having the same area as the tetrahedral triangle. Scaling with (55) gives $\lambda_1 = 4.949$ in excellent agreement.

A sector of the spherical cap making an angle φ has $A = \varphi(1-\cos\theta)$ and $L = \varphi\sin\theta + 2\theta$. Choosing the reference domain to be such a sector on the half-sphere that has $M_0(z) = z^{1+\frac{\pi}{\varphi}}(1-z^2)^{-1}\left(1 - z^{\frac{\pi}{\varphi}}\right)^{-1}$, $\gamma_0 = \nu_{01} = 1 + \frac{\pi}{\varphi}$, we get

$$\nu_1 = \frac{1}{2}\left(\cot\frac{\theta}{2} + \frac{\theta}{\varphi\sin^2\frac{\theta}{2}} - \frac{\pi}{\sqrt{2}\varphi\sin\frac{\theta}{2}} - 1\right) + \frac{\nu_{01}}{\sqrt{2}\sin\frac{\theta}{2}}. \tag{56}$$

Ratzkin and Treibergs [2009] present a theoretical result $\lambda_1 = 5.0046$ for the case $\varphi = \frac{2\pi}{3}$ and $\theta = \cos^{-1}\left(\frac{-1}{\sqrt{3}}\right)$ whereas the scaling procedure gives $\lambda_1 = 5.1046$.

As a domain on the sphere is shrunk retaining its shape, it tends to approximate a flat domain in the limit, allowing for a comparison to the available solutions on flat domains. For instance, as the spherical cap has its radius $\theta \to \delta \sim 0$, its $\nu_1 \to (1+\sqrt{2})\delta^{-1} = 2.4142\delta^{-1}$ that compares well with the flat disk solution $\sqrt{\lambda_1} = j_{0,1}\delta^{-1} = 2.4048\delta^{-1}$ ($j_{0,1}$ being the first zero of the Bessel function J_0). The second one $\nu_2 \sim (1+2\sqrt{2})\delta^{-1} = 3.8284\delta^{-1}$ also compares well with $\sqrt{\lambda_2} = j_{1,1}\delta^{-1} = 3.8317\delta^{-1}$. The next one $\nu_3 \sim 5.2426$ is close to $\sqrt{\lambda_3} = 5.1356$. As expected, higher ones start showing up significant differences.

Complete solution on the equilateral triangle on the plane was obtained by Lamé [1833]. Comparing the octant triangle on the sphere, one finds for the equilateral triangle of side length δ on the plane $\nu_1 \sim \left(2\sqrt{3} + 2\sqrt{\frac{2\pi}{\sqrt{3}}}\right)\delta^{-1} = 7.273\delta^{-1}$ that compares well with Lamé's result $\sqrt{\lambda_1} = \frac{4\pi}{\sqrt{3}}\delta^{-1} = 7.255\delta^{-1}$. The second one $\nu_2 \sim \left(2\sqrt{3} + 4\sqrt{\frac{2\pi}{\sqrt{3}}}\right)\delta^{-1} = 11.083\delta^{-1}$ also compares well with $\sqrt{\lambda_2} = \frac{4\pi\sqrt{7}}{3}\delta^{-1} = 11.082\delta^{-1}$. The next one $\nu_3 \sim 14.892$ is close to $\sqrt{\lambda_3} = 14.510$. Here too, higher ones start showing up significant differences.

More generally, one can use the flat domain solution to estimate the first few eigenvalues on a similar domain on the sphere. Given A and L for a domain Ω^2 on the sphere and A_0 and L_0 for a similar domain Ω_0^2 on the plane, one finds for $\nu_k, k = 1, 2, \cdots$ on Ω^2,

$$\nu_k = \frac{1}{2}\left(\frac{L}{A} - \frac{L_0}{\sqrt{AA_0}} - 1\right) + \sqrt{\frac{A_0\lambda_{0k}}{A}}, \tag{57}$$

where $\lambda_{0k}, k = 1, 2, \cdots$ are the eigenvalues of the Laplacian on Ω_0^2. This may be viewed as providing a curvature correction to the flat space eigenvalues. Note that the length scale on Ω_0^2 cancels out, and that A, L and ν_1 are in units set by the unit sphere.

Viewed as an extension of scaling of the Laplacian eigenvalues on flat domains to include curvature effects, the discrepancies in the scaling estimates could become significant as domains get too large relative to say the half-sphere. Also, the linear scaling procedure based on just two parameters is not expected to yield good results for all the eigenvalues, but its potential to do so for the first few is intriguing, especially because it is based on the first two coefficients of the series that governs the growth of the spectrum at large eigenvalues. Better results can be obtained with improved scaling estimates involving more parameters to match other coefficients in the series such as a quadratic scaling procedure discussed in the appendix. It will be interesting to study the applicability of a similar scaling procedure to the spectrum of other differential operators, or to more general domains extended to a cone or by taking (44) as defining $M(z)$. Also, of interest to study is the concept of factorizability of domains arising from the independence of particle subsystems, that is, from the separability of the solutions to the heat equation.

A Extended Scaling Procedure

The linear scaling estimate (48) with its two parameters is able to match the first two coefficients of the series expansion (38). It is helpful to have it extended to involve three parameters capable of matching the third coefficient of the series as well. The following derives such an extension making use of the heat kernel expansion on the sphere. Towards this end, consider the expansion for $M\left(e^{-s}\right)$,

$$M\left(e^{-s}\right) \simeq \frac{b_0}{s^{n-1}} + \frac{b_1}{s^{n-2}} + \frac{b_2}{s^{n-3}} + \cdots. \tag{58}$$

This gives rise to an expansion for the counting function $W(\nu)$ of the kind (46),

$$W(\nu) \simeq \frac{b_0 \nu^{n-1}}{(n-1)!} + \frac{b_1 \nu^{n-2}}{(n-2)!} + \frac{b_2 \nu^{n-3}}{(n-3)!} + \cdots. \tag{59}$$

We already know b_0 and b_1, and b_2 is yet to be determined. A convenient approach to deriving a scaling procedure without affecting multiplicities is to require the counting function to agree for the two comparison domains. The first two terms can be together approximated for large ν as $\sim \frac{b_0}{(n-1)!}(\nu+p)^{n-1}$ where $p = \frac{b_1}{b_0}$. To this order, one then obtains the scaling procedure (48) as a scaling of the linear combination $\nu + p$. To include the next order term, let us look for a quadratic combination $(\nu+p)^2 + q$ for some p and q such that, for large ν, $W(\nu)$ can be approximated as

$$W(\nu) \sim \frac{b_0}{(n-1)!}\left[(\nu+p)^2 + q\right]^{\frac{n-1}{2}}. \tag{60}$$

Expanding this and comparing the coefficients, one finds

$$p = \frac{b_1}{b_0}, \quad q = (n-2)\left(\frac{2b_2}{b_0} - p^2\right). \tag{61}$$

To determine b_2, consider the heat kernel expansion on the sphere,

$$\mathrm{Tr} e^{t\nabla_S^2} \simeq (4\pi t)^{-\frac{n-1}{2}}\left(a_0 + a_1\sqrt{t} + a_2 t + \cdots\right). \tag{62}$$

The a-coefficients of this expansion are well-known (see for instance Vassilevich [2003]), the first three of which are

$$a_0 = \left|\Omega^{n-1}\right|, \quad a_1 = -\frac{\sqrt{\pi}}{2}\left|\partial\Omega^{n-1}\right|, \quad a_2 = \frac{1}{6}\int_{\Omega^{n-1}} R + \frac{1}{3}\int_{\partial\Omega^{n-1}} K. \tag{63}$$

Here $R = (n-1)(n-2)$ is the scalar curvature of S^{n-1} and hence that of Ω^{n-1}, and K is the trace of the extrinsic curvature of the boundary $\partial\Omega^{n-1}$ relative to Ω^{n-1}. Use of this expansion in the identity (44) rewritten as

$$M\left(e^{-s}\right) = \frac{e^{\ell s}}{\sqrt{\pi}}\int_0^\infty \frac{dt}{\sqrt{t}} e^{-t-\frac{\ell^2 s^2}{4t}} \mathrm{Tr} e^{\frac{s^2}{4t}\nabla_S^2}, \tag{64}$$

where $\ell = \frac{1}{2}(n-2)$, gives us the b-coefficients that yields

$$p = \ell - \frac{\gamma}{2}, \quad q = -\ell^2 - \frac{1}{4}(n-2)\gamma^2 + \frac{a_2}{\left|\Omega^{n-1}\right|}, \tag{65}$$

where γ is as defined in (40). Thus, given p and q as above, $(\nu+p)^2+q$ for a domain Ω^{n-1} can be estimated as β^2 times the same combination for a reference domain Ω_0^{n-1}. Scaling factor β is the same as before given by (49).

The quadratic scaling procedure thus defined is quite general applicable to domains with smooth boundaries. It can also be used on domains without boundaries in which case it becomes a linear procedure applied to the eigenvalues of the Laplacian itself. On the sphere, it can be used for instance on a spherical cap on S^{n-1} ($K=(n-2)\cot\theta$, where θ is its radius in angles), but it turns out to be identical to the linear procedure in the case of the spherical cap on S^2. For domains that have corners on their boundaries, the procedure is applicable with additional contributions to a_2 coming from corner regions of dimension $n-3$. On a triangular domain on S^2, each vertex of angle φ on the boundary contributes $\frac{1}{6}\left(\frac{\pi^2}{\varphi}-\varphi\right)$ to a_2 (making use of a result attributed to Kac [1966] that can be inferred in the present framework from the trace of the heat kernel on the $n=2$ cone following the discussion at the end of section 4). For our earlier numerical comparisons, this extended procedure offers the improvements: $\lambda_1 = 5.1625 \to 5.1606$ for the tetrahedral triangle, $\lambda_1 = 5.1046 \to 5.0187$ for the sector of a spherical cap and $\sqrt{\lambda_1} = 7.2734\delta^{-1} \to 7.2613\delta^{-1}$ for the equilateral triangle on the plane.

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