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Arkiv for Det Fysiske Seminar i Trondheim

No 11 - 1968

On certain Toeplitz-like matrices and their relation
to the problem of lattice vibrations*

by

Mark Kac**

PHYSICAL SCIENCES

JAN 28 1969

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*Based on a lecture given at the Trondheim Theoretical Physics Seminar on September 13, 1968.

**Address: Rockefeller University, New York, N.Y. 10021, U.S.A.

1° Consider a one dimensional chain of harmonic oscillators coupled by springs of equal strength but with possibly differing masses. Allowing for nearest neighbor interactions only, the Hamiltonian of the system is

$$H \equiv \sum_1^N \frac{p_k^2}{2m_k} + \frac{\kappa^2}{2} \sum_1^{N-1} (x_{k+1} - x_k)^2 . \quad (1.1)$$

As is well known the frequencies of the normal modes $\omega_1, \omega_2, \dots, \omega_N$ can be obtained by solving the determinantal equation

$$\Delta_N = \begin{vmatrix} 2-m_1\omega^2, & -\kappa^2, & 0, & 0, & \dots, & 0 \\ & -\kappa^2, & 2-m_2\omega^2, & -\kappa^2, & 0, & \dots, & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0, & 0, & 0, & \dots, & -\kappa^2, & 2-m_N\omega^2 \end{vmatrix} = 0 \quad (1.2)$$

and that if our chain is in thermal equilibrium at absolute temperature T then the (quantum-mechanical) partition function is

$$\begin{aligned} Q_N &= \prod_{s=1}^N \sum_{n=0}^{\infty} e^{-(n+\frac{1}{2})\hbar\omega_s/kT} \\ &= e^{-\frac{1}{2} \sum_{s=1}^N \hbar\omega_s/kT} \prod_{s=1}^N \frac{1}{1 - e^{-\hbar\omega_s/kT}} \\ &= e^{-\frac{1}{2} \sum_{s=1}^N \hbar\omega_s/kT} e^{\sum_{s=1}^N \log(1 - e^{-\hbar\omega_s/kT})} \end{aligned} \quad (1.3)$$

Let $NH_N(\omega)$ be the number of frequencies ω_s which are smaller than ω i.e.

$$H_N(\omega) = \frac{1}{N} \sum_{\omega_s < \omega} 1. \quad (1.4)$$

Then we have

$$Q_N = e^{-\frac{N}{2} \frac{\hbar}{kT} \int_0^{\infty} \omega dH_N(\omega)} e^{N \int_0^{\infty} \log(1 - e^{-\hbar\omega/kT}) dH_N(\omega)}.$$

If as $N \rightarrow \infty$ we have

$$H_N(\omega) \rightarrow H(\omega) \quad (1.5)$$

(in the usual sense of convergence of distribution functions) then we obtain in the thermodynamic limit ($N \rightarrow \infty$) the following formula for the free energy ψ per mode

$$-\frac{\psi}{kT} = -\frac{\hbar}{2kT} \int_0^{\infty} \omega dH(\omega) + \int_0^{\infty} \log(1 - e^{-\hbar\omega/kT}) dH(\omega). \quad (1.6)$$

Thus the thermodynamic properties of our chain will be completely determined if we know the spectral distribution function $H(\omega)$ or, if H is absolutely continuous, the spectral density

$$G(\omega) = \frac{dH}{d\omega} \quad (1.7)$$

2°. We shall consider in the sequel two cases

- (a) The "continuous case" in which $m_k = m\left(\frac{k}{N}\right)$, where $m(t)$ is a reasonably smooth function

and

- (b) The "purely random case" in which m_1, m_2, \dots, m_N are independent random variables having the same distribution function $R(m)$ so that

$$\text{Prob} \left\{ m_k < m \right\} = R(m) \quad .$$

The "continuous case" has been solved in even a more general setting by Kac, Murdock and Szegö [1], but we shall present here a different derivation because it is of some independent interest and because it is closely related to the approach we shall propose for dealing with the much more difficult case (b).

Let us first of all choose units so that $\kappa^2=1$ and note that for $\xi > 0$ (more generally $\text{Re}\xi > 0$)

$$D_N(m_1, m_2, \dots, m_N; \xi) =$$

$$\begin{vmatrix} 2+m_1\xi & -1 & 0 & \dots & 0 \\ -1 & 2+m_2\xi & -1 & \dots & 0 \\ 0 & -1 & 2+m_3\xi & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & -1 & 2+m_N\xi \end{vmatrix} \quad (2.1)$$

$$= m_1 m_2 \dots m_N \prod_{s=1}^N (\xi + \omega_s^2) \quad .$$

It follows immediately that

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{N} \log D_N &= \lim_{N \rightarrow \infty} \frac{\log m_1 + \dots + \log m_N}{N} + \\ &+ \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{s=1}^N \log(\xi + \omega_s^2) \quad (2.2) \\ &= \int_0^1 \log m(t) dt + \int_0^\infty \log(\xi + \omega^2) dH(\omega) \end{aligned}$$

and since $H(\omega)$ can (in principle) be determined from the transform

$$\int_0^\infty \log(\xi + \omega^2) dH(\omega)$$

(see e.g. Dyson [2]) we see that all we need is the limit

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log D_N .$$

If $m(t)$ is Riemann integrable it follows from a result in [1] that

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{N} \log D_N &= \\ &= \int_0^1 dt \frac{1}{2\pi} \int_{-\pi}^{\pi} \log(2 + \xi m(t) - 2 \cos \theta) d\theta , \quad (2.3) \end{aligned}$$

whence

$$\begin{aligned} \int_0^\infty \log(\xi + \omega^2) dH(\omega) &= \\ \int_0^1 dt \frac{1}{2\pi} \int_{-\pi}^{\pi} \log \left[\xi + \frac{2(1 - \cos \theta)}{m(t)} \right] d\theta \quad (2.4) \end{aligned}$$

and consequently

$$H(\omega) = \frac{1}{2\pi} \mu \left\{ \sqrt{\frac{2(1-\cos\theta)}{m(t)}} < \omega \right\}, \quad (2.5)$$

where μ denotes the ordinary (Lebesgue) measure of the set defined inside the braces, with the understanding that $0 \leq t \leq 1$ and $-\pi \leq \theta < \pi$.

To see how (2.3) comes about we start with the familiar formula

$$\frac{1}{\sqrt{D_N}} = \frac{1}{(\sqrt{\pi})^N} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{1}{2} \sum_{k=1}^N m_k x_k^2} e^{-\frac{1}{2} \sum_{k=1}^{N-1} (x_{k+1} - x_k)^2} dx_1 \dots dx_N \quad (2.6)$$

and setting

$$K_1(x, y) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2} \xi m_1 x^2} e^{-(x-y)^2} e^{-\frac{1}{2} \xi m_{1+1} y^2} \quad (2.7)$$

we see that

$$\begin{aligned} \frac{1}{\sqrt{D_N}} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} e^{-\frac{1}{2} \xi m_1 x_1^2} K_1(x_1, x_2) K_2(x_2, x_3) \dots \\ \dots K_{N-1}(x_{N-1}, x_N) e^{-\frac{1}{2} \xi m_N x_N^2} dx_1 \dots dx_N. \end{aligned} \quad (2.8)$$

Instead of the familiar situation in which a fixed kernel is iterated we have here a situation in which the kernel changes as it is being iterated.

Let us first assume that $m(t)$ is a step function. In other words let us assume that the interval $(0, 1)$ is divided into intervals $\Delta_1, \Delta_2, \dots, \Delta_r$ (which together

exhaust $(0,1)$) and that

$$m(t) = m^{(k)} \quad \text{if } t \text{ is in } \Delta_k, \quad k = 1, 2, \dots, r. \quad (2.9)$$

If we set now

$$K_{(1)}(x, y) = \frac{1}{\sqrt{\pi}} e^{-\frac{1}{2}m^{(1)}\xi x^2} e^{-(y-x)^2} e^{-\frac{1}{2}m^{(1)}\xi y^2}$$

we see from (2.8) that the kernel $K_{(1)}$ is iterated $N|\Delta_1|$ times ($|\Delta_k|$ denotes the length of Δ_k); the kernel $K_{(2)}$ is iterated $N|\Delta_2|$ times etc.

It is now easy to convince oneself (and the rigor is easily supplied) that for large N one has

$$\frac{1}{\sqrt{D_N}} \sim C \lambda_{(1)}^{N|\Delta_1|} \lambda_{(2)}^{N|\Delta_2|} \dots \lambda_{(r)}^{N|\Delta_r|} \quad (2.10)$$

where $\lambda_{(1)}$ is the maximum eigenvalue of $K_{(1)}$ and the constant C is of order 1 and comes from connecting different iterates across the discontinuities.

It therefore follows that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log D_N = -2 \sum_{k=1}^r |\Delta_k| \log \lambda_{(k)} = -2 \int_0^1 \log \lambda(t) dt, \quad (2.11)$$

where $\lambda(t)$ is the maximum eigenvalue of the kernel

$$\frac{1}{\sqrt{\pi}} e^{-\frac{1}{2}m(t)\xi x^2} e^{-(y-x)^2} e^{-\frac{1}{2}m(t)\xi y^2}. \quad (2.12)$$

Observing that the principal eigenfunction is of the form $\exp(-by^2)$ one obtains easily that

$$\lambda(t) = \left(\frac{2 + \xi m(t) + \sqrt{(2 + \xi m(t))^2 - 4}}{2} \right)^{-\frac{1}{2}}, \quad (2.13)$$

and consequently

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log D_N = \int_0^1 \log \left(\frac{2 + \xi m(t) + \sqrt{(2 + \xi m(t))^2 - 4}}{2} \right) dt. \quad (2.14)$$

This is equivalent to (2.3) since, as it is easily checked,

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \log(2 + \xi m - 2 \cos \theta) d\theta = \log \frac{2 + \xi m + \sqrt{(2 + \xi m)^2 - 4}}{2}.$$

Having proved (2.3) for step functions it is an easy matter to extend it to arbitrary Riemann integrable functions.

All one has to do is to recall that for every $\varepsilon > 0$ and every Riemann integrable $m(t)$ one can choose two step functions $m_\varepsilon^+(t)$ and $m_\varepsilon^-(t)$ such that

$$m_\varepsilon^-(t) \leq m(t) < m_\varepsilon^+(t)$$

and

$$\int_0^1 (m_\varepsilon^+(t) - m_\varepsilon^-(t)) dt < \varepsilon.$$

From (2.6) one sees then that $D_N^{-\frac{1}{2}}$ for $m(t)$ is contained between, $D_N^{-\frac{1}{2}}$ for $m_\varepsilon^+(t)$ (from below) and $D_N^{-\frac{1}{2}}$ for $m_\varepsilon^-(t)$ (from above).

If one assumes that $m(t)$ is twice differentiable with bounded $m''(t)$ then much more can be proved (see a note of ours "Asymptotic behaviour of a class of determinants" to

appear in a forthcoming volume of Enseignement Mathématique dedicated to the memory of Jean Karamata where we use an extension of the method described here, or a paper by Mejlbo and Schmidt in Mat.Scand. 10 (1962) pp.5-16 where a much more general result is proved by an entirely different method).

3°. Much more difficult and also more interesting is the "purely random" case. Here no wholly satisfactory solution exists although much progress has been made since Dyson's pioneering paper [2]. The most important contributions are reprinted in Lieb and Mattis, "Mathematical Physics in One Dimension" and interesting numerical results can be found in [3] and [4].

Here we propose yet another approach but warn the reader that an important point of rigor is left unsettled.

It would be more convenient to introduce the periodic boundary condition so that the Hamiltonian is

$$H = \sum_1^N \frac{p_k^2}{2m_k} + \frac{1}{2} \sum_1^N (x_{k+1} - x_k) \quad , \quad x_{N+1} = x_1 \quad ,$$

and the determinant D_N has to be modified by inserting -1 in the upper right and in the lower left corners.

Of interest now in the average spectral distribution

$$\langle H_N(\omega) \rangle$$

(3.1)

and we now have

$$\frac{1}{N} \langle \log D_N \rangle = \langle \log m \rangle + \int_0^{\infty} \log(\xi + \omega^2) d\langle H_N(\omega) \rangle \quad (3.2)$$

Hopefully

$$\langle H_N(\omega) \rangle \rightarrow \tilde{H}(\omega) \quad (3.3)$$

and, as before,

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle \log D_N \rangle = \langle \log m \rangle + \int_0^{\infty} \log(\xi + \omega^2) d\tilde{H}(\omega) \quad (3.4)$$

It should be understood that the average (mathematical expectation) is to be taken in accord with statistical assumptions which we make about the joint distribution of m_1, m_2, \dots, m_N . The simplest assumption is that the masses are independent random variables having the same joint distribution $R(u)$ i.e.

$$\text{Prob.} \{ m_k < u \} = R(u) \quad (3.5)$$

The most interesting case is the binomial case

$$R(u) = \int_0^u [p\delta(x-m) + q\delta(x-M)] dx \quad (3.6)$$

with

$$p + q = 1, \quad p > 0, \quad q > 0.$$

4°. We begin again with formula (2.6), except that $\sum_1^{N-1} (x_{k+1} - x_k)^2$ is replaced now by $\sum_1^N (x_{k+1} - x_k)^2$.

Taking averages of both sides and using independence of the m 's we obtain

$$\left\langle \frac{1}{\sqrt{D_N}} \right\rangle = \frac{1}{(\sqrt{\pi})^N} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \langle e^{-\xi m x_1^2} \rangle \dots \langle e^{-\xi m x_N^2} \rangle e^{-\frac{1}{2} \sum_1^N (x_{k+1} - x_k)^2} dx_1 \dots dx_N, \quad (4.1)$$

and we have therefore

$$\left\langle \frac{1}{\sqrt{D_N}} \right\rangle = \sum_{j=1}^{\infty} \lambda_j^N(1) \quad (4.2)$$

where the $\lambda_j(1)$ are the eigenvalues (in decreasing order) of the kernel

$$K_{(1)}(x, y) = \frac{1}{\sqrt{\pi}} \sqrt{G(\xi x^2)} e^{-(y-x)^2} \sqrt{G(\xi y^2)} \quad (4.3)$$

and

$$G(\xi x^2) = \langle e^{-\xi m x^2} \rangle = \int_0^{\infty} e^{-\xi m x^2} dR(x). \quad (4.4)$$

It is an easy exercise to extend (4.2) and to obtain for $k = 2, 3, \dots$

$$\left\langle \left(\frac{1}{\sqrt{D_N}} \right)^k \right\rangle = \sum_{j=1}^{\infty} \lambda_j^N(k)$$

where again the $\lambda_j(k)$ are the eigenvalues (in decreasing order) but of the k -dimensional kernel

$$K_{(k)}(\vec{x}, \vec{y}) = \frac{1}{(\sqrt{\pi})^k} \sqrt{G(\xi \|\vec{x}\|^2)} e^{-\|\vec{y}-\vec{x}\|^2} \sqrt{G(\xi \|\vec{y}\|^2)} \quad (4.6)$$

where $\|\vec{x}\|$ denotes the k -dimensional Euclidean length of the vector \vec{x} .

We have therefore, asymptotically,

$$\left\langle \left(\frac{1}{\sqrt{D_N}} \right)^k \right\rangle \sim \lambda_1^N(k) \quad (4.7)$$

for $k = 1, 2, 3, \dots$ and the first question is, can one extend (4.7) to non-integral exponents k ?

Since for integral k the principal eigenfunction is of spherical symmetry one checks easily that $\lambda_1(k)$ is also the maximum eigenvalue of the kernel

$$L_k(r, \rho) = \frac{2}{\sqrt{\pi}} r^{\frac{k-1}{2}} \rho^{\frac{k-1}{2}} e^{-(r^2 + \rho^2)} \sqrt{G(\xi r^2) G(\xi \rho^2)} \sum_{l=0}^{\infty} \frac{\Gamma(1 + \frac{l}{2})}{(2l)! \Gamma(1 + \frac{l}{2})} (2r\rho)^{2l}. \quad (4.8)$$

In this form the kernel is perfectly well defined and even Hilbert-Schmidt for all $k > 0$.

Its maximum eigenvalue is also perfectly well defined and we conjecture that for all $k > 0$ and large N

$$\left\langle \left(\frac{1}{D_N} \right)^k \right\rangle \sim \lambda_1^N(k) \quad (4.9)$$

with the understanding that, of course, now $\lambda_1(k)$ is the maximum eigenvalue of the kernel (4.8).

The conjecture appears to us extremely reasonable

because for the simple chain of equal masses,

$$G(\xi r^2) = e^{-m\xi r^2},$$

it can be trivially verified. It would be quite strange if for

$$G(\xi r^2) = pe^{-m\xi r^2} + qe^{-M\xi r^2}, \quad p+q = 1,$$

it were to fail as soon as either p or q became different from 0.

Still we have no rigorous proof.

As a partial (and very weak) check we can mention that as $k \rightarrow 0$

$$\lambda_1(k) \rightarrow 1.$$

This is easily shown by using the inequality

$$e^{-\xi m_{\max} r^2} \leq G(\xi r^2) \leq e^{-\xi m_{\min} r^2}.$$

If the conjecture (4.9) is correct and if, as seems likely, one has

$$\lambda_1(k) = 1 - \alpha k + \dots \quad (\alpha > 0) \quad (4.10)$$

for small positive k we obtain (formally) that

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle \log D_N \rangle = 2\alpha \quad (4.11)$$

and the whole problem is therefore reduced to finding α .

It would be of considerable interest to investigate the relationship between our approach and the approach of Dyson [2] and Schmidt [5].

5°. We conclude with a brief account of an abortive attempt to approach the Ising model by a method based on path integrals. Since the main difficulties are already present in the one-dimensional case we shall restrict ourselves to this case only.

We write the usual partition function of the one-dimensional Ising model in the form

$$Q_N = e^{-aN} \sum_{\vec{\mu}} e^{-a \sum_{k=1}^N \mu_k^2 + \nu \sum_{k=1}^{N-1} \mu_k \mu_{k+1}} \quad (5.1)$$

where a is sufficiently large to make the quadratic form

$$a \sum_1^N \mu_k^2 - \nu \sum_1^{N-1} \mu_k \mu_{k+1}$$

positive definite (in other words $a > \nu$) and ν , as usual, is given by the formula

$$\nu = \frac{J}{kT} \quad (5.2)$$

We rewrite Q_N in the form

$$Q_N = e^{-aN} \int_{-\infty}^{\infty} \dots \int e^{-a \sum \mu_k^2 + \nu \sum \mu_k \mu_{k+1}} \prod_1^N \delta(\mu_k^2 - 1) d\mu_1 \dots d\mu_N \quad (5.3)$$

and using the standard representation of the δ -function

$$\delta(\mu^2-1) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi(\mu^2-1)} d\xi$$

we obtain in a few steps

$$Q_N = \frac{e^{-aN}}{(2\sqrt{\pi})^N} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \frac{e^{-i(\xi_1+\dots+\xi_N)}}{\begin{vmatrix} a-i\xi_1, & -\frac{\nu}{2}, & 0, \dots, 0 \\ -\frac{\nu}{2}, & a-i\xi_2, & -\frac{\nu}{2}, & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ 0, & 0, \dots, & -\frac{\nu}{2}, & a-i\xi_N \end{vmatrix}}^{\frac{1}{2}} d\xi_1 \dots d\xi_N \quad (5.4)$$

The square root of the determinant in the denominator above causes no difficulty as long as $a > \nu$. It is now tempting to hope that $\xi_1, \xi_2, \dots, \xi_N$ can be thought of as "lying along a curve" i.e. we think of ξ_k as being $\xi(k/N)$ where $\xi(t)$, $0 \leq t \leq 1$, is a reasonably "smooth" function.

If this is so then by a slight extension of the result discussed in §2 the denominator of the integrand in (5.4) is asymptotically

$$\exp \left[-\frac{N}{2\pi} \frac{1}{2} \int_0^1 dt \int_{-\pi}^{\pi} \log(a-i\xi(t) - \nu \cos \theta) d\theta \right] \quad (5.5)$$

and the numerator is, of course, (again asymptotically)

$$e^{-N \int_0^1 \xi(t) dt} \quad (5.6)$$

One can be still more optimistic and hope that the integral in (5.4) is a discretization of a "path integral" so that one may rewrite (5.4) in the form

$$Q_N \approx \frac{e^{-aN}}{(2\sqrt{\pi})^N} \int_e \left\{ -i \int_0^1 \xi(t) dt - \frac{1}{4\pi} \int_0^1 dt \int_{-\pi}^{\pi} \log(a - i\xi(t) - v \cos \theta) d\theta \right\} d(\text{path}) . \quad (5.7)$$

One can now attempt the method of steepest descent in the space of paths.

This leads to the variational equation

$$\delta \left\{ -i \int_0^1 \xi(t) dt - \frac{1}{4\pi} \int_0^1 dt \int_{-\pi}^{\pi} \log(a - i\xi(t) - v \cos \theta) d\theta \right\} = 0$$

and the only smooth solution is $\xi(t) \equiv \text{const.}$

It then turns out that since $\xi(t)$ must be real a must be chosen in an essentially unique way and we finally end up with the same result as that given by the spherical model [6].

We have committed so many "crimes" that it is only just that we have been "punished" by a wrong answer. Perhaps the only surprising thing is that the answer is not wholly absurd and, in part, quite reasonable for high temperature.

The main "crime" is no doubt the one pointed out many years ago by the late T.H. Berlin namely that the ξ_k 's "lie along a smooth curve".

Perhaps the failure of this attempt is one more reminder that nature tends to be unkind to the mathematician, a profound observation first made by Fourier.

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Appendix to "On certain Toeplitz-like matrices and their relation to the problem of lattice vibrations" by Mark Kac. (Arkiv for Det Fysiske Seminar i Trondheim, No 11 - 1968).

After a lecture I gave at Cornell University based on the material of the Trondheim lecture, Professor Kenneth G. Wilson of the Physics Department of Cornell University has found a simple and elegant way of calculating α (see (4.10)). With Professor Wilson's permission I shall reproduce his calculation.

We start by writing

$$L_k(r, \rho) = \frac{2}{\Gamma(\frac{k}{2})} f_k(r) f_k(\rho) + M_k(r, \rho), \quad (A.1)$$

where

$$f_k(r) = r^{\frac{k-1}{2}} e^{-r^2} \sqrt{G(\xi r^2)} \quad (A.2)$$

and

$$M_k(r, \rho) = \frac{2}{\sqrt{\pi}} r^{\frac{k-1}{2}} \rho^{\frac{k-1}{2}} e^{-r^2} e^{-\rho^2} \sqrt{G(\xi r^2)} \sqrt{G(\xi \rho^2)} \sum_{l=1}^{\infty} \frac{\Gamma(1 + \frac{1}{2})}{(2l)! \Gamma(1 + \frac{k}{2})} (2r\rho)^{2l}. \quad (A.3)$$

Let now $u_n^{(k)}(r)$ and $\lambda_n^{(k)}$ be the normalized eigenfunctions and eigenvalues of the kernel $M_k(r, \rho)$. The kernel $M_k(r, \rho)$ can be easily seen to be positive definite and we have

by Mercer's theorem

$$M_k(r, \rho) = \sum_{n=1}^{\infty} \lambda_n^{(k)} u_n^{(k)}(r) u_n^{(k)}(\rho). \quad (\text{A.4})$$

Let $\lambda_1(k)$ be the largest eigenvalue of L_k and let ψ be the corresponding eigenfunction.

Since $u_n^{(k)}$ form a complete set we can expand ψ and f_k in them obtaining

$$\begin{aligned} \psi(\rho) &\sim \sum \psi_n u_n^{(k)}(\rho) \\ f_k(\rho) &\sim \sum f_n^{(k)} u_n^{(k)}(\rho). \end{aligned} \quad (\text{A.5})$$

Note also that as long as $k > 0$ $f_k(\rho) \in L^2(0, \infty)$ so that the standard L^2 theory is applicable.

Since ψ is an eigenfunction of L_k , and $\lambda_1(k)$ the corresponding eigenvalue, we have (using (A.4) and the first formula in (A.5)) that

$$\lambda_1(k)\psi(r) = \frac{2}{\Gamma(\frac{k}{2})} f_k(r) \int_0^{\infty} f_k(\rho)\psi(\rho)d\rho + \sum_{n=1}^{\infty} \lambda_n^{(k)} \psi_n u_n^{(k)}(r). \quad (\text{A.6})$$

Multiplying both sides of (A.6) by $u_n^{(k)}(r)$ and integrating we obtain

$$\lambda_1(k)\psi_n = \frac{2}{\Gamma(\frac{k}{2})} f_n^{(k)} \int_0^{\infty} f_k(\rho)\psi(\rho)d\rho + \lambda_n^{(k)} \psi_n$$

or

$$\psi_n = \frac{2}{\Gamma(\frac{k}{2})} \frac{f_n^{(k)}}{\lambda_1(k) - \lambda_n^{(k)}} \int_0^{\infty} f_k(\rho)\psi(\rho)d\rho. \quad (\text{A.7})$$

Using now Parseval's relation

$$\int_0^{\infty} f_k(\rho)\psi(\rho)d\rho = \sum_{n=1}^{\infty} \psi_n f_n^{(k)}$$

we obtain almost at once that

$$1 = \frac{2}{\Gamma(\frac{k}{2})} \sum_{n=1}^{\infty} \frac{f_n^{(k)^2}}{\lambda_1(k) - \lambda_n^{(k)}} \quad (A.8)$$

Use has been made of the obvious fact that

$$\int_0^{\infty} f_k(\rho)\psi(\rho)d\rho \neq 0 \quad (A.9)$$

Formula (A.8) can now be rewritten in the equivalent form

$$\lambda_1(k) = \frac{2}{\Gamma(\frac{k}{2})} \sum_{n=1}^{\infty} f_n^{(k)^2} + \frac{2}{\Gamma(\frac{k}{2})} \sum_{n=1}^{\infty} \frac{\lambda_n^{(k)} f_n^{(k)^2}}{\lambda_1(k) - \lambda_n^{(k)}}$$

and since

$$\begin{aligned} \sum_{n=1}^{\infty} f_n^{(k)^2} &= \int_0^{\infty} f_k^2(r)dr = \\ &= \int_0^{\infty} r^{k-1} e^{-2r^2} G(\xi r^2)dr = \\ &= \left[p(2+\xi m)^{\frac{k}{2}} + q(2+\xi M)^{\frac{k}{2}} \right] \frac{1}{2} \Gamma(\frac{k}{2}) \end{aligned}$$

we have

$$\lambda_1(k) = p(2+\xi m)^{\frac{k}{2}} + q(2+\xi M)^{\frac{k}{2}} + \frac{2}{\Gamma(\frac{k}{2})} \sum_{n=1}^{\infty} \frac{\lambda_n^{(k)} f_n^{(k)^2}}{\lambda_1(k) - \lambda_n^{(k)}} \quad (A.10)$$

If we now let $k \rightarrow 0$ (through positive values) we see

immediately that

$$\lambda_1(k) \sim 1 - \frac{k}{2} [p \log(2+\xi m) + q \log(2+\xi M)] + k \sum_{n=1}^{\infty} \frac{\lambda_n}{1-\lambda_n} f_n^2$$

where the λ_n 's are the eigenvalues of the kernel

$$M_0(r, \rho) = 2 \frac{e^{-r^2}}{\sqrt{r}} \frac{e^{-\rho^2}}{\sqrt{\rho}} \sqrt{G(\xi r^2)} \sqrt{G(\xi \rho^2)} \sum_{l=1}^{\infty} \frac{(r\rho)^{2l}}{l!(l-1)!} \quad (\text{A.11})$$

and

$$f_n = \int_0^{\infty} \frac{1}{\sqrt{r}} \sqrt{G(\xi r^2)} u_n(r) dr, \quad (\text{A.12})$$

the $u_n(r)$ being the (normalized) eigenfunctions of M_0 .

Thus (by (4.11))

$$\lim_{N \rightarrow \infty} \frac{1}{N} \langle \log D_N \rangle = 2\alpha = p \log(2+\xi m) + q \log(2+\xi M) - 2 \sum_{n=1}^{\infty} \frac{\lambda_n}{1-\lambda_n} f_n^2. \quad (\text{A.13})$$

This is as explicit a formula as one can get but whether it can be usefully discussed remains to be seen.

We conclude by showing how (A.10) can be extended to

$$k = -2.$$

We write the infinite sum in (A.10) in the form

$$\begin{aligned} \frac{2}{\Gamma(\frac{k}{2})} \sum_{r=1}^{\infty} \sum_{n=1}^{\infty} \left[\frac{\lambda_n^{(k)}}{\lambda_1^{(k)}} \right]^r f_n^{(k)^2} &= \frac{2}{\Gamma(\frac{k}{2})} \frac{1}{\lambda_1^{(k)}} \sum_{n=1}^{\infty} \lambda_n^{(k)} f_n^{(k)^2} + \\ &+ \frac{2}{\Gamma(\frac{k}{2})} \sum_{r=2}^{\infty} \sum_{n=1}^{\infty} \left[\frac{\lambda_n^{(k)}}{\lambda_1^{(k)}} \right]^r f_n^{(k)^2} = \\ &= \frac{2}{\Gamma(\frac{k}{2})} \frac{1}{\lambda_1^{(k)}} \int_0^{\infty} \int_0^{\infty} \hat{r}_k(r) M_k(r, \rho) f_k(\rho) dr d\rho + \end{aligned}$$

$$+ \frac{2}{\Gamma(\frac{k}{2})} \sum_{r=2}^{\infty} \sum_{n=1}^{\infty} \left[\frac{\lambda_n^{(k)}}{\lambda_1^{(k)}} \right]^r f_n^{(k)2} .$$

It is easy to convince oneself that as $k \rightarrow -2$ only the first of the two terms above survives (i.e. does not approach 0). In fact, only the first term of M_k yields a non-vanishing contribution and we have as $k \rightarrow -2$

$$\lambda_1(-2) = p(2+\xi m) + q(2+\xi M)$$

$$+ \frac{1}{\lambda_1(-2)} \lim_{k \rightarrow -2} \frac{2}{\Gamma(\frac{k}{2})} \int_0^{\infty} \int_0^{\infty} f_k(r) M_k(r, \rho) f_k(\rho) dr d\rho = 2 + \xi \langle m \rangle +$$

$$+ \frac{1}{\lambda_1(-2)} \lim_{k \rightarrow -2} \frac{2}{\Gamma(\frac{k}{2})} \frac{2}{\Gamma(1 + \frac{k}{2})} \left[\int_0^{\infty} r^{k+1} e^{-2r^2} G(\xi r^2) dr \right]^2$$

$$= (2 + \xi \langle m \rangle) - \frac{1}{\lambda_1(-2)} ,$$

where

$$\langle m \rangle = pm + qM$$

is the average mass.

We have thus obtained a quadratic equation for $\lambda_1(-2)$

and

$$\lambda_1(-2) = \frac{2 + \xi \langle m \rangle + \sqrt{(2 + \xi \langle m \rangle)^2 - 4}}{2} . \quad (\text{A.14})$$

Let us recall that we have conjectured that

$$\left\langle \left(\frac{1}{\sqrt{D_N}} \right)^k \right\rangle \sim \lambda_1^N(k) \quad (\text{A.15})$$

holds for all positive k . It now appears that the conjecture is verified even for $k = -2$! For in this case the direct calculation of $\langle D_N \rangle$ shows that it is equal to the determinant (2.1) with all masses replaced by the average mass $\langle m \rangle$ and this elementary determinant is asymptotically

$$\lambda_1^N(-2)$$

with $\lambda_1(-2)$ given by (A.14).