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Measuring the insulating ability of anisotropic thermal conductors via principal Dirichlet eigenvalue

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We consider the thermal insulation property of homogeneous anisotropically heat-conducting bodies, i.e. those whose thermal tensor (matrix) A is constant throughout the body but not generally a constant times the identity. This anisotropy is a common feature of *nano-composite* materials. We propose using the principal Dirichlet eigenvalue λ of the associated elliptic differential operator $-\nabla \cdot A\nabla$ as a simple measurement for the insulating ability of the material, because the time scale of thermal flow is of the order of $1/\lambda$. $1/\lambda$ is a generalization of the 'R-value' used in engineering practice as a measure of the insulating ability of *isotropic* conductors. If the thermal tensor A depends on parameters, e.g. inherited from nanostructure, then so does λ. It is important to know how λ depends on the parameters. For the material to be a good insulator, λ should be suppressed. But calculation or estimation of this principal elliptic eigenvalue, particularly over *ranges* of parameter values, is not a simple task. The focus of this paper is estimation – by fitted formulas and new exact bounds – of the principal elliptic Dirichlet eigenvalue of ellipses (2D) and ellipsoids (3D) *using only* simple expressions in the eigenvalues of the matrix A. Our simplest approximations and bounds avoid even the calculation of matrix eigenvalues and use in 2D merely the trace and determinant of A, and in 3D the trace and determinant of A and the trace of A^2. The new bounds are shown to imply an extremal property in homogenization theory and a new condition for enhancement in Taylor dispersion. Recently, Zheng, Forest, Lipton, Zhou and Wang published formulas for the thermal tensor A in the case of strong extensional fiber-type flow of a polymer with dilute rod-like nano-inclusions, including explicitly the influence of the probability distribution of inclusion orientation. Our results are combined with these formulas to quantify the effect of variations of the probability distribution on the insulating ability of the composite.

1 Introduction

In engineering practice, for isotropic materials, the 'R-value' (the reciprocal of the scalar heat-conductivity coefficient) is used to measure insulating ability. In case of anisotropic

materials, we propose using the principal Dirichlet eigenvalue λ_1 of the unit ball B_1 occupied by the homogeneous, anisotropic material as a simple measurement for the same thing. To be precise, let $A = (a_{ij})$ be the thermal tensor of an anisotropic but homogeneous material, and consider the Dirichlet eigenvalue problem:

$$\begin{cases} \nabla \cdot (A\nabla u) + \lambda u = 0 & \text{in } B_1 \\ u = 0 & \text{on } \partial B_1. \end{cases}$$

Let $\lambda(B_1)$ be the principal Dirichlet eigenvalue. If the material is isotropic, i.e. $A = kI$ with I the identity matrix, then $\lambda(B_1)$ is proportional to k, and as we can see in the eigen expansion of the corresponding heat equation, $1/\lambda(B_1)$ is the order of the time scale of thermal flow at the centre of the material. Thus, $\lambda(B_1)$ is a good (and simple) indicator of the thermal insulation property, and $1/\lambda(B_1)$ is a natural generalization of the R-value.

Anisotropy is a common feature of *nano-composite* materials – when isotropic nanoscale periodic structure is averaged out by the process of homogenization, the resulting effective thermal diffusion is generally anisotropic [2, 4]. If the thermal tensor A (positive-definite, symmetric) depends on parameters, perhaps inherited from nanostructure (volume fraction of inclusions, orientation parameters and the like – see, for example, the expression for the thermal tensor in the recent paper [8]) then so does $\lambda(B_1)$. It is important to know how $\lambda(B_1)$ depends on the parameters. For the material to be a good insulator, $\lambda(B_1)$ should be suppressed.

The reason for selecting the ball as standard reference shape is its invariance under rotations. The Dirichlet eigenvalues (principal and higher) inherit this invariance. Consequently, the Dirichlet eigenvalues are functions only of the rotational invariants of the thermal matrix: the trace and determinant and in 3D also the trace of A^2. The Dirichlet eigenvalues are linear homogeneous functions of A of degree 1. There are no explicit (much less, simple and useable) analytic formulas for these eigenvalues; although in 2D, there are (highly non-explicit) formulas involving Mathieu functions.

The focus of this paper is estimation – by fitted formulas and new exact bounds – of the principal elliptic Dirichlet eigenvalue $\lambda(B_1)$ *using only* simple expressions in the eigenvalues of the matrix A. Our simplest approximations and bounds avoid even the calculation of matrix eigenvalues and use in 2D merely the trace and determinant of A and in 3D the trace and determinant of A and the trace of A^2. These are done in Sections 2 and 3. (By stretching the coordinate system, we can handle the principal eigenvalue of elliptical domains, and thus at the beginning of Sections 2 and 3, the eigenvalue problem is formulated on ellipses and ellipsoids.)

The new bounds are applied in Section 2 to 2D Taylor dispersion and in Section 3 to demonstrate a new extremal property in 3D homogenization theory. In Section 4, our results are combined with the explicit formulas in ref. [8] to quantify the effect of varying nano-parameters, particularly those of the probability distribution of inclusion orientation, on the insulating ability of the composite.

Our results, of course, also apply to the study of principal *vibration frequencies* of ellipses and ellipsoids.

Two of us have recently studied the practical problem of protecting an isotropic conductor (e.g. a space shuttle) from overheating by an anisotropic coating, establishing an easy-to-use rule for the optimal thickness of the coating required (see [6]).

2 Principal eigenvalue of an ellipse (2D)

We consider the Dirichlet eigenvalue problem (principal eigenvalue and eigenfunction) for $-\nabla \cdot (A\nabla)$ in an elliptical region in 2D:

$$\begin{cases} a_{11}u_{xx} + 2a_{12}u_{xy} + a_{22}u_{yy} + \lambda u = 0 & x^2/\alpha^2 + y^2/\beta^2 < 1 \\ u = 0 & x^2/\alpha^2 + y^2/\beta^2 = 1, \end{cases} \tag{1}$$

where α and β are positive constants and $A = (a_{ij})$ is a constant symmetric positive-definite 2×2 matrix.

Introduce scaled coordinates $\bar{x} = x/\alpha$ and $\bar{y} = y/\beta$. Then the problem becomes the Dirichlet eigenvalue problem (principal eigenvalue remains the same) for $-\nabla \cdot (\bar{A}\nabla)$ in the unit disc, where

$$\bar{A} = \begin{pmatrix} a_{11}/\alpha^2 & a_{12}/(\alpha\beta) \\ a_{12}/(\alpha\beta) & a_{22}/\beta^2 \end{pmatrix},$$

i.e.

$$\begin{cases} \bar{a}_{11}u_{\bar{x}\bar{x}} + 2\bar{a}_{12}u_{\bar{x}\bar{y}} + \bar{a}_{22}u_{\bar{y}\bar{y}} + \lambda u = 0 & \bar{x}^2 + \bar{y}^2 < 1 \\ u = 0 & \bar{x}^2 + \bar{y}^2 = 1. \end{cases}$$

Rotating coordinates to diagonalize $\bar{A}$ (the domain is now rotationally invariant), we find that this principal Dirichlet eigenvalue $\lambda(\bar{A})$ is the same as the principal Dirichlet eigenvalue $\lambda(a, b)$ of the operator $-a\frac{\partial^2}{\partial x^2} - b\frac{\partial^2}{\partial y^2}$, where $a > 0$ and $b > 0$ are the eigenvalues of the matrix $\bar{A}$:

$$\begin{cases} au_{xx} + bu_{yy} + \lambda(a, b)u = 0 & x^2 + y^2 < 1 \\ u = 0 & x^2 + y^2 = 1. \end{cases} \tag{2}$$

These new coordinates should really be called $\bar{\bar{x}}$ and $\bar{\bar{y}}$, but here and in the next step we do not bother with this.

Exact bounds. Let $t = a/b = \epsilon^2 \leqslant 1$. As a function of t, λ is analytic in $t > 0$, increasing and $d^2\lambda/dt^2 \leqslant 0$. (This concavity and the use of it to obtain bounds go back to Polya and Schiffer [5] and Weinberger [7], who also explicitly discussed elliptical domains.) Hence the graph of λ versus t lies between the secant line joining $(0, \lambda(0))$ and $(1, \lambda(1))$ and the tangent line at $t = 1$. Analytically, this implies[1] (see [7])

$$\frac{\pi^2}{4}b + \left(5.783186 - \frac{\pi^2}{4}\right)a \leqslant \lambda(\bar{A}) \leqslant \frac{1}{2}\,5.783186(a + b) \quad a < b,$$

[1] Recall that 5.783186 is (approximately) the principal Dirichlet eigenvalue of $-\Delta$ on the unit disc.

i.e.

$$2.4674011b + 3.3157849a \leqslant \lambda(\bar{A}) \leqslant 2.891593(a+b) \quad a < b.$$

The above implies a cruder lower bound in terms of trace alone:

$$2.4674011 \cdot \mathrm{tr}(\bar{A}) \leqslant \lambda(\bar{A}) \leqslant 2.891593 \cdot \mathrm{tr}(\bar{A}).$$

We also recall the well-known Faber–Krahn inequality, which states that the first Dirichlet eigenvalue of $-\Delta$ on any bounded domain in n-dimensional space is no less than that of the ball with the same volume. Thus,

$$\begin{aligned}\lambda(\bar{A}) &= \lambda(a,b)\\ &\geqslant \frac{5.783186}{1/\sqrt{ab}}\\ &= 5.783186\sqrt{\det(\bar{A})}.\end{aligned}$$

This is a better lower bound only when a and b are close, $1 > \epsilon > 0.744$.

Fitted (trace/determinant) approximations. Two examples of what we shall define (below) as *trace/determinant* approximations are the following:

$$\lambda(\bar{A}) = 2.515631 \cdot \mathrm{tr}(\bar{A}) + 0.800155 \cdot \sqrt{\det \bar{A}} \pm 0.04824\|\bar{A}\|, \tag{3}$$

and

$$\begin{aligned}\lambda(\bar{A}) = {} & 2.445735 \cdot \mathrm{tr}(\bar{A}) + 0.248073 \cdot \sqrt{\det \bar{A}}\\ & + 0.470443 \cdot \sqrt[4]{\det(\bar{A})} \cdot \sqrt{\mathrm{tr}(\bar{A})} \pm 0.02167\|\bar{A}\|.\end{aligned} \tag{4}$$

The numerical coefficients in these equations are the results of *fittings* to be explained below. The matrix norm $\|\bar{A}\|$ is the largest eigenvalue of $\bar{A}$. Note that apart from the error estimates, these two formulas for the elliptic eigenvalues *avoid even the calculation of matrix eigenvalues, since the trace and determinant are known immediately from the thermal tensor*. (The same will be true of the corresponding approximation in 3D; although in the application we make of this to nano-composites, it happens that the eigenvalues of the effective tensor are simple to write down.)

Derivation of (3). Dividing equation (2) by b, we find

$$\lambda(a,b) = b\lambda(\epsilon), \tag{5}$$

where

$$\epsilon = \sqrt{\frac{a}{b}}, \tag{6}$$

so that $\lambda(\epsilon)$ is the principal Dirichlet eigenvalue of

$$\begin{gathered}\epsilon^2 u_{xx} + u_{yy} + \lambda u = 0 \quad x^2 + y^2 \leqslant 1 \\ \Updownarrow \\ \Delta u + \lambda u = 0 \quad \epsilon^2 x^2 + y^2 \leqslant 1.\end{gathered}$$

Since $\lambda(a, b) \equiv \lambda(b, a)$, $\lambda(\epsilon)$ must satisfy

$$\lambda(\epsilon) = \epsilon^2 \lambda(1/\epsilon) \quad \epsilon > 0. \tag{7}$$

The following evaluations are well known:

- $\lambda(0) = \pi^2/4 \approx 2.4674011$.
- $\lambda(1) = a_1^2 \approx 5.783186$, where a_1 is the first positive zero of the Bessel function J_0.

We seek approximations to $\lambda(\epsilon)$ satisfying (7) (call solutions of (7) *invariants*). Generally,

- for any function f, the expression $F(\epsilon) \equiv f(\epsilon) + \epsilon^2 f(1/\epsilon)$ is an invariant.
- If F and G are invariants, so is $F^\gamma \cdot G^\nu$ for any $\gamma \geqslant 0$ and $\nu \geqslant 0$ satisfying $\gamma + \nu = 1$.
- Any linear combination of invariants is an invariant.

Taking $f \equiv 1$ we find the invariant $1 + \epsilon^2$, and taking $f(\epsilon) = \epsilon$ we find the invariant ϵ. Therefore, the following is invariant:

$$(1 + \epsilon^2)^\gamma \cdot \epsilon^\nu \quad \gamma \geqslant 0, \quad \nu \geqslant 0, \quad \gamma + \nu = 1. \tag{8}$$

Multiplying by a and setting $\epsilon = \sqrt{b/a}$ (see (5) and (6)), we find the expression

$$(\mathrm{tr}(\bar{A}))^\gamma \cdot (\det(\bar{A}))^{\nu/2},$$

which means that approximations to $\lambda(\epsilon)$ that are linear combinations of terms of the form (8) give rise to approximations for $\lambda(\bar{A})$ that

- depend (in a very simple way) only on trace and determinant of $\bar{A}$
- and are homogeneous functions of degree 1 of the entries of $\bar{A}$.

These we call *trace/determinant* approximations, and we have found that approximations of this form are surprisingly accurate. Approximation (3) is a linear combination of two terms only, with $\gamma = 1$ and $\gamma = 0$. Approximation (4) includes one more term, with $\gamma = 1/2$. *Let c_1 and c_2 be the unique constants minimizing the absolute error* in the approximation of type (3)

$$E = \min_{c_1, c_2} \max_{0 \leqslant \epsilon \leqslant 1} |\lambda(\epsilon) - c_1(1 + \epsilon^2) - c_2 \epsilon|. \tag{9}$$

Hence,

$$\begin{aligned}\lambda(\epsilon) &= c_1(1 + \epsilon^2) + c_2 \epsilon \pm E \quad 0 \leqslant \epsilon \leqslant 1 \\ &\equiv p(\epsilon) \pm E \quad 0 \leqslant \epsilon \leqslant 1,\end{aligned}$$

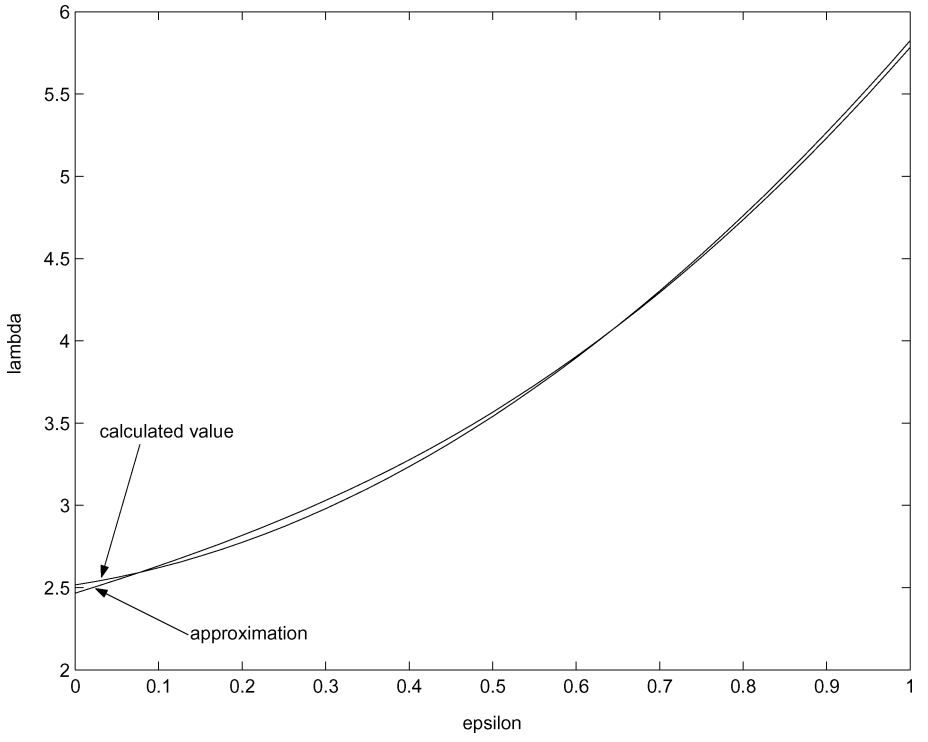

FIGURE 1. Eigenvalue curve $\lambda(\epsilon)$ and the fitted approximation $2.51563(1+\epsilon^2)+0.800155\epsilon$.

defining $p(\epsilon)$ (see Figure 1). Now using (7), we find

$$\begin{aligned}\lambda(\epsilon) &= \begin{cases} p(\epsilon) \pm E & 0 < \epsilon < 1 \\ \epsilon^2 p(1/\epsilon) \pm E\epsilon^2 & \epsilon > 1 \end{cases} \\ &= \begin{cases} p(\epsilon) \pm E & 0 < \epsilon < 1 \\ p(\epsilon) \pm E\epsilon^2 & \epsilon > 1 \end{cases} \\ &= p(\epsilon) \pm E \max(1, \epsilon^2).\end{aligned}$$

Now using (5), we find

$$\begin{aligned}\lambda(a,b) &= b\lambda(\epsilon) \\ &= bp(\epsilon) \pm E \max(b, \epsilon^2 b) \\ &= bp(\epsilon) \pm E \max(a,b) \\ &= c_1(a+b) + c_2\sqrt{ab} \pm E \max(a,b)\end{aligned}$$

which explains (3) except for the substitution of numerical values for c_1, c_2 and E. For this purpose a database of close approximations $\lambda_{\text{app}}(\epsilon)$, $0 \leqslant \epsilon \leqslant 1$ was created using finite differences (a small database was published in [3]) and then the L^∞-fitting algorithm

of Barrodale-Phillips [1] was applied. The result is $c_1 \approx 2.515631$, $c_2 \approx .800155$ and $E \approx .04824$. □

The above derivation is appealing, but we could have simply reasoned that the principal elliptic eigenvalue λ of $-\nabla \cdot (A\nabla)$ inherits the rotational symmetry of the domain (a disc) and so must be a function of the (two) rotational invariants of A. It must also be a homogeneous function of degree 1 of A ($A \to \alpha A$ implies $\lambda \to \alpha\lambda$ for $\alpha > 0$). The trace is already homogeneous of degree 1 and we take the square root of the determinant to obtain a form that is homogenous of degree 1. In 3D we will take this route.

Application of lower bound to 2D Taylor dispersion. *Taylor dispersion* (see [2]) refers to the effective enhancement of diffusion as $\epsilon \downarrow 0$ in the advection–diffusion equation

$$\frac{\partial T}{\partial t} + \frac{1}{\epsilon}\mathbf{v}(\mathbf{x}/\epsilon) \cdot \nabla T = \Delta T,$$

where $\mathbf{v}$ is a periodic, incompressible, mean-zero flow. Homogenization of this equation shows that T is approximated by anisotropic heat flow with thermal tensor

$$A = \begin{pmatrix} 1 + \langle |\nabla F_1|^2 \rangle & \langle \nabla F_1 \cdot \nabla F_2 \rangle \\ \langle \nabla F_1 \cdot \nabla F_2 \rangle & 1 + \langle |\nabla F_2|^2 \rangle \end{pmatrix},$$

where F_1 and F_2 are solutions of certain elliptic boundary value problems over the period cell and $\langle Q \rangle$ denotes the mean of Q over the cell. Accordingly, enhancement of diffusion should be identified with enhancement of the principal Dirichlet eigenvalue $\lambda(A)$ of $-\nabla \cdot (A\nabla)$ on the unit disc, i.e.

$$\lambda(A) > 5.78.$$

But the lower bound just derived is

$$\lambda(A) \geqslant \frac{\pi^2}{4}(2 + \langle |\nabla F_1|^2 \rangle + \langle |\nabla F_2|^2 \rangle).$$

Hence in terms of the cell problem, *a sufficient condition for enhancement of dispersion is*

$$\langle |\nabla F_1|^2 \rangle + \langle |\nabla F_2|^2 \rangle > 0.34.$$

3 Principal eigenvalue of an ellipsoid (3D)

Let $A = (a_{ij})$ be a 3×3 positive-definite constant matrix. Now we study the principal Dirichlet eigenvalue λ of $\sum a_{ij}u_{ij} + \lambda u = 0$ in an ellipsoidal domain

$$\frac{x^2}{\alpha_1^2} + \frac{y^2}{\alpha_2^2} + \frac{z^2}{\alpha_3^2} \leqslant 1.$$

As in 2D, this problem is reduced to the Dirichlet eigenvalue problem

$$au_{xx} + bu_{yy} + cu_{zz} + \lambda(a, b, c)u = 0,$$

for the unit ball B_1 in 3D ($x^2 + y^2 + z^2 \leqslant 1$) where a, b and c are the eigenvalues of the matrix

$$\bar{A} : (i, j) \mapsto \frac{a_{ij}}{\alpha_i \alpha_j}. \tag{10}$$

Fitted (trace, determinant, etc.) approximations. The fitted 3D approximations are motivated in the same way as in 2D. They will have one more term, corresponding to the quadratic term in the characteristic polynomial of the matrix $\bar{A}$, $(\mathrm{tr}(\bar{A}))^2 - \mathrm{tr}(\bar{A}^2)$; to make this term linear homogeneous of degree 1, we take the square root. The result is (If the middle invariant had been replaced by simply $\sqrt{\mathrm{tr}(\bar{A}^2)}$, the fitting would be slightly less accurate.)

$$\begin{aligned}\lambda_1 = {} & 2.5732131\mathrm{tr}(\bar{A}) + 0.442382663\sqrt{(\mathrm{tr}(\bar{A}))^2 - \mathrm{tr}(\bar{A}^2)} + 1.17216492\left(\det \bar{A}\right)^{1/3} \\ & \pm 0.1058||A||. \end{aligned} \tag{11}$$

As in 2D an accurate tabular database of Dirichlet eigenvalues versus matrix eigenvalues was created, but the 3D computation is much more demanding. We used two methods: finite differences (followed by Matlab's implementation of the LAPACK algorithms) and spectral collocation applied to the PDE expressed in spherical coordinates. The two methods agree very well and give rise to virtually the same fittings.

If the fitting is performed on any *subset* of the database, the accuracy is of course improved. One might know, for example, that of the three eigenvalues of the thermal tensor, the two smaller ones are equal. This leads to

$$\begin{aligned}\lambda = {} & 2.47626019\mathrm{tr}(\bar{A}) + 1.8918364\sqrt{(\mathrm{tr}(\bar{A}))^2 - \mathrm{tr}(\bar{A}^2)} - 2.2038579\det(\bar{A})^{1/3} \\ & \pm 0.0106||\bar{A}||. \end{aligned} \tag{12}$$

If the two *larger* eigenvalues of the thermal tensor are equal, then

$$\begin{aligned}\lambda_1 = {} & 2.4736805\mathrm{tr}(\bar{A}) + 0.550489306\sqrt{(\mathrm{tr}(\bar{A}))^2 - \mathrm{tr}(\bar{A}^2)} + 1.15745974\det(\bar{A})^{1/3} \\ & \pm .0573||\bar{A}|| \end{aligned} \tag{13}$$

Exact bounds.

Theorem 1 *Suppose the eigenvalues of the matrix* (10) *are* $a \leqslant b \leqslant c$. *Then*

$$4.0864a + 3.3158b + 2.4674c \leqslant \lambda(\bar{A}) \leqslant 3.2899(a + b + c).$$

Replacing 3.3158 and 4.0864 by 2.4674, we come to an inequality that is weaker but easier to apply since it avoids calculation of matrix eigenvalues.

Corollary 1 $2.4674 \cdot tr(\bar{A}) \approx \dfrac{\pi^2}{4} tr(\bar{A}) \leqslant \lambda(\bar{A}) \leqslant \dfrac{\pi^2}{3} tr(\bar{A}) \approx 3.2899 \cdot tr(\bar{A})$.

Remark 1 In 3D the lower bound provided by the Faber–Krahn inequality is

$$\lambda(\bar{A}) \geqslant \pi^2(abc)^{1/3} = \pi^2(\det(\bar{A}))^{1/3}.$$

Proof of Theorem 1 We use the ideas of ref. [7]. Observe that $\lambda(a,b,c) = b\lambda(a/b,1,c/b) = b\lambda(t,1,s)$, where $0 < t = a/b \leqslant 1 \leqslant s = c/b$.

By the variational characterization,

$$\lambda(t,1,s) = \inf_{u\in H_0^1(B_1),u\not\equiv 0} I(u),$$

where $I(u)$ is the Rayleigh quotient

$$I(u) = \frac{\int_{B_1} tu_x^2 + u_y^2 + su_z^2}{\int_{B_1} u^2}.$$

For fixed $u \in H_0^1(B_1)$, $I(u)$ is linear in t and s, and hence $\lambda(t,1,s)$, as the minimum of $I(u)$ over u, is concave in t and s. Thus for $0 < t \leqslant 1 \leqslant s$,

$$\begin{aligned}\lambda(t,1,s) &\geqslant \lambda(0,1,s) + (\lambda(1,1,s) - \lambda(0,1,s))\,t \\ &= \lambda(0,1,s)(1-t) + \lambda(1,1,s)t,\end{aligned}$$

where $\lambda(0,1,s)$ is understood as $\lim_{t\downarrow 0}\lambda(t,1,s)$, which is easily seen to be the first eigenvalue of

$$\begin{cases} u_{yy} + su_{zz} + \lambda u = 0 & D_1 := \{y^2 + z^2 < 1\} \\ u = 0 & \partial D_1. \end{cases}$$

By the 2D results

$$\begin{aligned}\lambda(0,1,s) &= s\lambda(0,1/s,1) \\ &\geqslant s\left(\frac{\pi^2}{4} + \left(5.783186 - \frac{\pi^2}{4}\right)(1/s)\right) \\ &= \frac{\pi^2}{4}(s-1) + 5.783186.\end{aligned}$$

On the other hand, by the concavity of $\lambda(\cdot,\cdot,1)$,

$$\begin{aligned}\lambda(1,1,s) &= s\lambda(1/s,1/s,1) \\ &\geqslant s[\lambda(0,0,1) + (\lambda(1,1,1) - \lambda(0,0,1))\,(1/s)] \\ &= s\left[\frac{\pi^2}{4} + \left(\pi^2 - \frac{\pi^2}{4}\right)(1/s)\right] \\ &= \frac{\pi^2}{4}(s-1) + \pi^2.\end{aligned}$$

Now

$$\lambda(t,1,s) \geqslant \left(\frac{\pi^2}{4}(s-1)+5.783186\right)(1-t)+t\left(\frac{\pi^2}{4}(s-1)+\pi^2\right)$$
$$=\left(5.783186-\frac{\pi^2}{4}\right)+(\pi^2-5.783186)t+\frac{\pi^2}{4}s.$$

This provides a lower bound for the unscaled eigenvalue

$$\lambda(a,b,c) = b\lambda(a/b,1,c/b)$$
$$\geqslant b\left[\left(5.783186-\frac{\pi^2}{4}\right)+(\pi^2-5.783186)(a/b)+\frac{\pi^2}{4}(c/b)\right]$$
$$=\left(5.783186-\frac{\pi^2}{4}\right)b+(\pi^2-5.783186)a+\frac{\pi^2}{4}c$$
$$=4.0864a+3.3158b+2.4674c.$$

To obtain an upper bound, we simply use the eigenfunction $(1/r)\sin\pi r$, $r=\sqrt{x^2+y^2+z^2}$, of $-\Delta$ on B_1 as a test function in the Rayleigh quotient, with the result

$$\lambda(a,b,c) \leqslant \frac{\pi^2}{3}(a+b+c)$$
$$=3.2899(a+b+c).$$

□

Application to 3D homogenization theory. Consider the heat equation $u_t=\nabla\cdot(k(\mathbf{x}/\epsilon)\nabla u)$, where k is periodic and $\epsilon\downarrow 0$. The homogenized equation (see [2]) is $u_t=\nabla\cdot(A\nabla u)$ where A (the effective diffusion tensor) is constant and is obtained by solving three *cell problems*, auxiliary elliptic problems in the period cell.

Corollary 2 *In 3D, among all periodic diffusion coefficients with cell average* $\langle k\rangle$ *equal to* $\beta>0$, *the one leading to the largest* $\lambda_1(-\nabla\cdot(A\nabla))$ *on the unit ball is the constant* $k(\mathbf{x}/\epsilon)\equiv\beta$.

Proof The proof depends on a simple fact about the formula for A: its diagonal elements are all less than or equal to $\langle k\rangle$. Hence

$$\lambda_1(-\nabla\cdot(k\nabla)) \to \lambda_1(-\nabla\cdot(A\nabla))$$
$$\leqslant \pi^2 tr(A)/3$$
$$\leqslant \pi^2(3\langle k\rangle)/3$$
$$=\pi^2\beta$$
$$=\lambda_1(-\beta\Delta).$$

□

4 Application to time scale of thermal flow in nano-composites

When explicit formulas for the thermal tensor A are available, the results discussed above lead to approximations and exact estimates of the principal Dirichlet eigenvalue of an elliptical body in terms of material nano-parameters.

By combining the homogenization method and the Doi–Hess kinetic theory, Zheng, Forest, Lipton, Zhou and Wang [8] obtained analytic formulas for the effective electrical conductivity tensor of nematic polymers with dilute nano-inclusions in the shape of spheroidal rods or platelets, and showed explicitly the dependence on the probability distribution of inclusion orientation. Since the effective *thermal* tensor can be obtained in exactly the same way, some of their results can be applied to the thermal (insulation) case except that now the thermal conductivity of the nano-inclusions is much less than that of the polymer background.

Consider a polymer body Ω, with dilute uniformly distributed nano-inclusions in the shape of high aspect-ratio spheroids with semi-axis lengths $a \gg b = c$, in the direction of unit vectors $\mathbf{m}$, $\mathbf{n}$ and $\mathbf{k}$, respectively. The inclusions are not assumed to be perfectly aligned: vector $\mathbf{m}$ is a random variable with given probability distribution function $f(\mathbf{m})$ for $\mathbf{m} \in S^2$. Let the volume fraction of inclusions be $\theta \ll 1$, and denote the thermal conductivities of the polymer background and inclusion by σ_p and σ_n, respectively, with *(strong) contrast parameter* $\sigma_n/\sigma_p \ll 1$. Then the effective thermal tensor (see [8, equation (12)]) is given by

$$A = \sigma_p I + \frac{(\sigma_n - \sigma_p)\sigma_p}{\sigma_n + \sigma_p - (\sigma_n - \sigma_p)L_a}\left[2I + \frac{(\sigma_n - \sigma_p)(1 - 3L_a)}{\sigma_p + (\sigma_n - \sigma_p)L_a}M\right]\theta + \mathrm{O}(\theta^2), \tag{14}$$

where I is the 3×3 identity, $L_a \ll 1$ is the *spheroidal depolarization factor* (see [8] for exact definition of L_a)

$$L_a \approx \frac{\log(r)}{r^2} \qquad r = a/b \gg 1, \tag{15}$$

and M is the covariance matrix

$$M_{ij} = E[m_i m_j] = \int_{S^2} m_i m_j f(\mathbf{m})\,\mathrm{d}S(\mathbf{m}). \tag{16}$$

Since the symmetric matrix A is a linear combination of the identity and M, M and A can be simultaneously diagonalized, so if the eigenvalues of M: d_1, d_2, d_3 are known, the eigenvalues of A: μ_1, μ_2, μ_3 can be read off from (14):

$$\mu_i = \sigma_p + \frac{(\sigma_n - \sigma_p)\sigma_p}{\sigma_n + \sigma_p - (\sigma_n - \sigma_p)L_a}\left[2 + \frac{(\sigma_n - \sigma_p)(1 - 3L_a)}{\sigma_p + (\sigma_n - \sigma_p)L_a}d_i\right]\theta + \mathrm{O}(\theta^2) \quad i = 1, 2, 3 \tag{17}$$

The values of d_i have to satisfy

$$0 \leqslant d_i \leqslant 1 \qquad d_1 + d_2 + d_3 = 1,$$

so we can parametrize them by

$$d_1 = \frac{1}{3} - w_1, \tag{18}$$

$$d_2 = \frac{1}{3} - w_2, \tag{19}$$

$$d_3 = \frac{1}{3} + w_1 + w_2, \tag{20}$$

where (w_1, w_2) must lie in the triangle T

$$T = \left\{ (u,v) | -\frac{2}{3} \leqslant u \leqslant \frac{1}{3}, -\frac{2}{3} \leqslant v \leqslant \frac{1}{3}, -\frac{1}{3} \leqslant u+v \leqslant \frac{2}{3} \right\}. \tag{21}$$

Substituting (18) into (17) and then these tensor eigenvalues μ_i into (11), we find a (complicated) expression approximating the principal Dirichlet eigenvalue λ_1 of the unit ball in 3D. Since we have assumed small values of θ, L_a and σ_n/σ_p, we calculate (using Mathematica) the second-degree Taylor polynomial of λ_1 with respect to these three variables centred at zero. The result is

$$\lambda_1/\sigma_p \approx 9.97 + \theta \left(-16.63 + 9.97 L_a + 29.93 \frac{\sigma_n}{\sigma_p} - 0.57\theta \left(w_1^2 + w_1 w_2 + w_2^2 \right) \right)$$
$$+ \text{cubics} + \cdots$$
$$= 9.97 - 16.63\theta + 9.97 L_a \theta + 29.93 \frac{\sigma_n}{\sigma_p}\theta - 0.57\theta^2 \left(w_1^2 + w_1 w_2 + w_2^2 \right). \tag{22}$$

There might be additional θ^2 terms; (14) was not fully established to that order in [8]. However, we can conclude that the values of w_1 and w_2 influence *only* the coefficient of θ^2 and possibly the coefficients of terms of degree $\geqslant 3$.[2]

Qualitative interpretation of (22)

- The last included term in (22) is negative

$$-0.57\theta^2 \left(w_1^2 + w_1 w_2 + w_2^2 \right), \tag{23}$$

hence contributes to the suppression of λ_1, and we may ask what is the *range* of suppression, i.e. to extremize $w_1^2 + w_1 w_2 + w_2^2$ in its domain T. We find

$$0 \leqslant w_1^2 + w_1 w_2 + w_2^2 \leqslant \frac{1}{3}$$

the minimum occurring at $w_1 = w_2 = 0$ (all eigenvalues of M equal $1/3$; distribution is uniform; medium is *optically isotropic*), and the maximum occurring at three points: $(-2/3, 1/3)$, $(1/3, -2/3)$, $(1/3, 1/3)$. All three of these correspond to the *smatic* case

[2] If $\mu_i \to \mu_i + r_i\theta^2$, then $\lambda_1 \to \lambda_1 + 3.33(\sum r_i)\theta^2$.

(perfect, non-random alignment of inclusions, the eigenvalues of M are 1, 0 and 0 of same order).

- Thus the probability distribution influences only quadratic and higher-degree terms in the expansion,
- always results in a suppression of λ_1, as far as quadratic terms are concerned
- and this suppression is maximized in the smatic case and minimized in the case of the uniform distribution.

- The remaining terms are

$$\lambda_1/\sigma_p \approx 9.97 + \theta\left(-16.63 + 9.97L_a + 29.93\frac{\sigma_n}{\sigma_p}\right). \tag{24}$$

At $\theta = 0$, there are no inclusions and we know $\lambda_1 = \pi^2\sigma_p$, which is consistent with the above result. The perturbation of this for $\theta > 0$ is proportional to θ and is largely a suppression. The suppression would be maximized by $L_a = \sigma_n/\sigma_p = 0$, which is impossible to realize. But if L_a and σ_n/σ_p are small, the suppression is near optimum. *Note that*

- *any increase in θ results in a 17-fold suppression of λ_1,*
- *any decrease in σ_n/σ_p results in a 30θ-fold suppression and*
- *any decrease in L_a results in a 10θ-fold suppression.*

- **Exact values of the first four coefficients in expansion of** λ_1. As we have pointed out, *the first four terms in the expansion of λ_1 are independent of w_1 and w_2*. Taking $w_1 = w_2 = 0$ makes $M = \frac{1}{3}I$ so $A = \alpha I$, a scalar multiple of the identity (with error $O(\theta^2)$ and cubic terms). Now if we assume aspect ratio high enough and contrast ratio small enough (*strong enough* contrast)

$$L_a < 0.05 \qquad \sigma_n/\sigma_p < 0.05 \tag{25}$$

then we can show, after lengthy estimates, that the coefficient α is given by

$$\alpha = \sigma_p + 2\theta\sigma_p\left[-1 + L_a + 2\frac{\sigma_n}{\sigma_p} - O_1\right] + \theta\sigma_p\left[1 - 3\frac{\sigma_n}{\sigma_p} - 3L_a + O_2\right](1/3) + O(\theta^2), \tag{26}$$

where O_1 and O_2 are small

$$0.3562\left(\frac{\sigma_n^2}{\sigma_p^2} + L_a^2\right) \leqslant O_1 \leqslant 0.9523\left(\frac{\sigma_n^2}{\sigma_p^2} + L_a^2\right), \tag{27}$$

$$0.8521\left(\frac{\sigma_n^2}{\sigma_p^2} + L_a^2\right) \leqslant O_2 \leqslant 7.7782\left(\frac{\sigma_n^2}{\sigma_p^2} + L_a^2\right). \tag{28}$$

Hence

$$\begin{aligned}\lambda_1/\sigma_p &\approx \pi^2\alpha \\ &\approx \pi^2\left(\sigma_p + 2\theta\sigma_p\left[-1 + L_a + 2\frac{\sigma_n}{\sigma_p}\right] + \theta\sigma_p\left[1 - 3\frac{\sigma_n}{\sigma_p} - 3L_a+\right](1/3)\right) \\ &= \pi^2 + \theta\left(-\frac{5}{3}\pi^2 + \pi^2 L_a + 3\pi^2\frac{\sigma_n}{\sigma_p}\right) \\ &\approx 9.87 + \theta\left(-16.45 + 9.87L_a + 29.61\frac{\sigma_n}{\sigma_p}\right).\end{aligned}$$

Our argument shows that the coefficients in the next-to-last equation are the exact *coefficients in the Taylor expansion of that order.*

Calculation of the θ^2-contribution to suppression of λ_1 in three cases. The θ^2-suppression term was

$$-0.57\theta^2\left(w_1^2 + w_1w_2 + w_2^2\right).$$

We shall consider three cases of orientation distribution from among the many studied in ref. [8]. Remember that there may be additional θ^2 terms unaccounted for.

Uniform distribution: $w_1 = w_2 = 0$, no quadratic suppression.

Smatic case – perfect alignment: $w_1 = w_2 = 1/3$, so quadratic suppression is $-0.19\theta^2$.

Weak steady shear': Before quenching, the material is subjected to a weak steady shear, therefore with Peclet number $\mathrm{Pe} \ll 1$ (a non-dimensional measurement of the shear rate). A parameter N is introduced

$$N = \frac{8r\theta}{\pi} \tag{29}$$

and we now need to assume (see [8])

$$\theta < \frac{1.9635}{r} - \frac{0.734}{r}\frac{r^2-1}{r^2+1}\mathrm{Pe}^{1/2} \tag{30}$$

which implies

$$N < 5 - 1.869\frac{r^2-1}{r^2+1}\mathrm{Pe}^{1/2} < 5. \tag{31}$$

In this case the eigenvalues of M computed in [8] are

$$\begin{aligned}d_1 &= \frac{1}{3} + \frac{\mathrm{Pe}}{6(N-5)} \\ d_2 &= \frac{1}{3} \\ d_3 &= \frac{1}{3} - \frac{\mathrm{Pe}}{6(N-5)}.\end{aligned}$$

leading to the quadratic suppression

$$-0.016\theta^2\left(\frac{\mathrm{Pe}}{N-5}\right)^2.$$

Using (30), we find *the maximum possible (quadratic) suppression for weak shear flow to be*

$$\approx -0.005\theta^2\mathrm{Pe}(1+r^{-2}). \tag{32}$$

Quiescent nematic case: [8, Section 5.3] Here

$$d_1 = \frac{1+2s}{3} \tag{33}$$

$$d_2 = d_3 = \frac{1-s}{3} \tag{34}$$

where

$$s = \frac{1}{4}\left(1+3\sqrt{1-\frac{8}{3N}}\right) \in \left(\frac{1}{4},1\right).$$

The resulting suppression is $-0.19\theta^2 s^2$ and lies in the range

$$-1.188\theta^2 < -0.19\theta^2 s^2 < -0.19\theta^2.$$

5 Conclusions

We aimed at finding a scalar measurement of the thermal insulation property of a homogeneous, anisotropically conducting material. We proposed that this be the first Dirichlet eigenvalue $\lambda_1(B_1)$ of the elliptic operator $-\nabla\cdot A\nabla$ on the unit ball composed of the material, where A is the thermal tensor of the material. The rationale for this choice is based on the eigen-expansion of the corresponding heat equation, and the fact that $1/\lambda_1(B_1)$ is the natural generalization of the R-value commonly used in the engineering practice for isotropically conducting materials.

Thus, for the material to be a good thermal insulator, $\lambda_1(B_1)$ needs to be suppressed.

The next pressing issue is to find a user-friendly approximate formula for $\lambda_1(B_1)$ in terms of A. In 2D, by the earlier work of Polya, Schiffer and Weinberger, $\lambda_1(B_1)$ can be bounded, reasonably well, in terms of the trace of A; however, in 3D, the rigorous bounds we have are not so satisfactory. So we established some numerically fitted formulas for $\lambda_1(B_1)$ involving in 2D only the trace and the determinant of A (and in 3D the trace of A^2): knowledge of the entire tensor A is not needed.

If formulas for the thermal tensor A are known, the above approximations can provide insights into the proper design of good insulators. We illustrated this point by studying the nano-composite materials whose thermal tensors were explicitly obtained in ref. [8]. We found, among other things, that when the nano-inclusions are perfectly aligned, $\lambda_1(B_1)$ is minimized, while when they are randomly oriented, $\lambda_1(B_1)$ is maximized. In other words, perfect alignment of nano-inclusions enhances the R-value, and hence the insulating ability of the material.

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