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Composite Homogenization via the Equivalent Poly-Inclusion Approach

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Abstract

The theory of the effective elastic response of biphase composite materials, with arbitrary second-phase geometry, concentration, and orientation distribution, is formulated in terms of the average inclusion strain concentrator for an entirely uniform body undergoing a uniform eigenstrain in a non-dilute family of morphologically identical internal regions (inclusions). Admissibility criteria for approximate inclusion strain concentrators are formulated. The relation of the present approach with the traditional one, based on the inhomogenity average strain concentrator, is investigated, and the current homogenization approaches are confirmed to be generally inadmissible. Finally, a family of fully admissible concentrators is proposed, together with the corresponding effective stiffness tensors.

1. INTRODUCTION

The 'effective' or 'equivalent' stiffness tensor $\underline{C}$ of a composite material is defined through the relation

$$\bar{\sigma} = \underline{C}\, \epsilon^{o}. \tag{1}$$

where ϵ^{o} is a homogeneous deformation applied at the boundary and $\bar{\sigma}$ is the resulting average stress.

For a biphase composite, consisting of a matrix of stiffness $\underline{C}^{m}$, containing a volumetric concentration α of inhomogeneities, or fibers, of stiffness $\underline{C}^{f}$, the effective stiffness may be exactly expressed as

$$\underline{C} = \underline{C}^{m} + \alpha < (\underline{C}^{f} - \underline{C}^{m})\, \underline{A} > \tag{2}$$

where the pointed brackets denote orientational averaging, weighted by a fiber orientation probability density function (Ferrari & Johnson, 1989). In equation (2), the (average) strain concentration tensor $\underline{A}$ was introduced. This is defined by the equation:

$$\bar{\epsilon}^{f} = \underline{A}\ \epsilon^{o} \tag{3}$$

where ϵ^{o} is as in (1), a superscript f refers to the fiber phase, and overbars denote spatial averaging.

Eshelby (1957) showed the strain concentrator for the limit case

of a composite consisting of a single anisotropic ellipsoidal inhomogeneity in an infinite matrix to be

$$\underline{T} = [\underline{I} + \underline{E} (\underline{C}^m)^{-1} (\underline{C}^f - \underline{C}^m)]^{-1} \qquad (4)$$

where $\underline{I}$ is the fourth rank symmetric identity tensor, and $\underline{E}$ is defined in eq. (8) below.

At non-dilute volumetric fiber concentrations, $\underline{T}$ is no longer an appropriate concentrator. The determination of the adequate concentrator $\underline{A}$ is essential, for the purpose of homogenization, in view of the fact that, once the fiber orientation profile and the tensor $\underline{A}$ are known, the homogenization problem is reduced to a mere computational exercise, according to (2). However, this tensor is not generally available, in the case of arbitrary fiber spacings and concentration levels. The need thus arises for introducing estimates for $\underline{A}$.

While the appropriateness of such estimates and the associated effective medium theories must be assessed experimentally, on a case-to-case basis, some physical considerations may guide the choice of the approximate expressions for the strain concentrator $\underline{A}$. In particular, the following are necessary conditions for the general validity of any homogenization scheme:

Requirement 1: The effective stiffness $\underline{C}$ must be diagonally symmetric. This ensures reversibility of any composite deformation in

the linear elastic range.

Requirement 2: In the power series expansion of $\underline{C}$ in terms of α, the first order term must be $< (\underline{C}^f - \underline{C}^m)\ \underline{T} >$. Requirement 2 ensures the recovery of Eshelby's exact solution at dilute concentrations.

Requirement 3: At the unitary fiber concentration limit, the effective stiffness prediction must be independent of the matrix properties.

Requirement 4: The effective moduli associated with $\underline{C}$ must comply with the variational bounds. Examples of such bounds are those obtained by Hashin and Shtrikman (1963) for macroscopically isotropic composites with isotropic phases.

No currently available homogenizing approach complies with all of these admissibility criteria, for arbitrarily specified second-phase geometry, anisotropy, and orientation distribution. In particular: Voigt's (1928) assumption $\underline{A} = \underline{I}$ violates Requirements 2 and 4, while Eshelby's (1957) assumption $\underline{A} = \underline{T}$ violates Requirements 3 and 4. The Mori-Tanaka approach (1973), based on the assumption

$$\underline{A} = \underline{T}\ [(1-\alpha)\ \underline{I} + \alpha\ <\underline{T}>]^{-1} \qquad (5)$$

complies with the Requirements 1 and 3 if and only if the inhomogeneities are perfectly aligned, or consist of isotropic material (Ferrari, 1991).

In the present paper, effective medium theory is reformulated in

the context of an equivalent eigenstraining poly-inclusion problem. In the new formulation, the poly-inclusion strain concentrator $\hat{\underline{E}}$, defined in (9), replaces $\underline{A}$ as the independent variable of the homogenizing scheme. This affords a considerably simplified analytical statement of the physical admissibility requirements. Subsequently, a family of fully admissible homogenization approaches is explicitly identified, and some examples are discussed.

2. THE EQUIVALENT EIGENSTRAINING POLY-INCLUSION PROBLEM.

To solve the problem of the single ellipsoidal inhomogeneity in an infinite matrix subject to the uniform boundary strain ϵ^0, Eshelby (1957) devised to substitute the inohomogeneity with an equal volume Ω of matrix material (the 'inclusion'), subject to a uniform eigenstrain ϵ^* of unknown amount. This unknown equivalent eigenstrain was then calculated from the condition that the inhomogeneity and its equivalent eigenstraining inclusion be equally stressed:

$$\mathbf{C}^f(\epsilon^0 + \epsilon^c) = \mathbf{C}^m(\epsilon^0 + \epsilon^c - \epsilon^*) \quad \text{in } \Omega \tag{6}$$

Here, ϵ^c is the strain perturbation due to Ω. This procedure then reduced the single inhomogeneity problem to the previously solved the problem of a large homogenous body with uniform non-zero eigenstraining in Ω only.

Eshelby (1957) proceeded to determine that the strain in the

inhomogeneity is uniform, and given by

$$\epsilon^{f} = \bar{\epsilon}^{f} = \underline{T}\, \epsilon^{o} \tag{7}$$

in duality with the fact that the strain in the equivalent eigenstraining inclusion is uniform, and given by

$$\epsilon^{\Omega} = \bar{\epsilon}^{\Omega} = \underline{E}\, \epsilon^{*} + \epsilon^{o} \tag{8}$$

For the general poly-inhomogeneity case, relation (7) must be approximated by (3). Similarly, the average inclusion strains for the case of a non-dilute concentration of inclusions, undergoing the same uniform eigenstrain ϵ^{*} and in the absence of mechanical loads is not given by (8). In this context, the approximate expression

$$\bar{\epsilon}^{\Omega} = \hat{\underline{E}}\, \epsilon^{*} \tag{9}$$

is now introduced, in analogy with (3). By paralleling Eshelby's original developments, the poly-inclusion and the poly-inhomogeneity problems are put in correspondence by imposing that the average inhomogeneity stress and the average inclusion stress coincide. Consequently, the inhomogeneity average strain in the non-dilute case is

$$\bar{\epsilon}^f = \hat{\underline{T}}\, \epsilon^0 \tag{10}$$

with corresponding approximate effective stiffness

$$\underline{C} = \underline{C}^m + \alpha < (\underline{C}^f - \underline{C}^m)\, \hat{\underline{T}} > \tag{11}$$

where $\hat{\underline{T}}$ is obtained from $\underline{T}$ by replacing $\underline{E}$ with $\hat{\underline{E}}$ in (4).

3. ADMISSIBILITY CRITERIA - A FAMILY OF ADMISSIBLE CONCENTRATORS

In the following, the poly-inclusion strain concentrator $\hat{\underline{E}}$, rather than $\underline{A}$, is employed as the governing quantity of the homogenization scheme. The relation between these tensors is

$$\hat{\underline{E}} = (\underline{A}^{-1} - \underline{I})\, (\underline{C}^f - \underline{C}^m)^{-1}\, \underline{C}^m \tag{12}$$

as is found by equating (2) and (11).

To analytically express the symmetry condition, requirement number 1 above, it is first realized that $\underline{C}$ is symmetric if and only if the contraction $(\underline{C}^f - \underline{C}^m)\, \hat{\underline{T}}$ is. However, by the definition of $\hat{\underline{T}}$,

$$\begin{aligned}(\underline{C}^f - \underline{C}^m)\, \hat{\underline{T}} &= (\underline{C}^f - \underline{C}^m)\, [\underline{I} + \hat{\underline{E}}\, (\underline{C}^m)^{-1}\, (\underline{C}^f - \underline{C}^m)\,]^{-1} = \\ &\{\, [\underline{I} + \hat{\underline{E}}\, (\underline{C}^m)^{-1}\, (\underline{C}^f - \underline{C}^m)\,]\, (\underline{C}^f - \underline{C}^m)^{-1}\,\}^{-1} = \\ &\{\, (\underline{C}^f - \underline{C}^m)^{-1} + \hat{\underline{E}}\, (\underline{C}^m)^{-1}\,\}^{-1}\end{aligned} \tag{13}$$

Thus, it is concluded that $\underline{C}$ is symmetric if and only if $\hat{\underline{E}}\ (\underline{C}^m)^{-1}$ is.

Requirement number 2 is equivalent to imposing that the limit of $\hat{\underline{E}}$ as α approaches zero be Eshelby's tensor $\underline{E}$. Requirement number 3 may be equivalently expressed by the condition that

$$\underline{C}_1 \equiv \underline{C}^m + \langle [(\underline{C}^f - \underline{C}^m)^{-1} + \hat{\underline{E}}\ (\underline{C}^m)^{-1}]^{-1} \rangle \tag{14}$$

be matrix independent for all composites. Here, $\underline{C}_1$ and $\hat{\underline{E}}_1$ denote the unitary concentration limits of $\underline{C}$ and $\hat{\underline{E}}$, respectively. For a void second-phase, (14) reduces to

$$\underline{C}_1 = \underline{C}^m \langle \underline{I} + (\hat{\underline{E}}_1 - \underline{I})^{-1} \rangle = \underline{C}^m \langle \hat{\underline{E}}_1\ (\hat{\underline{E}}_1 - \underline{I})^{-1} \rangle. \tag{15}$$

In order for $\underline{C}_1$ to vanish, regardless of the matrix properties, it is thus necessary that

$$\langle \hat{\underline{E}}_1\ (\hat{\underline{E}}_1 - \underline{I})^{-1} \rangle = 0. \tag{16}$$

Since no quantity in (16) depends on $\underline{C}^f$, the holding of (16) for all composites is equivalent to requirement 3. Further specialization of (16) is possible, considering the special case of perfectly second-phase alignment. In this context, the orientational averagings may be deleted, and (16) is equivalent to

$$\hat{\underline{E}}_1 = 0. \tag{17}$$

For texture-independent $\hat{\underline{E}}$, requirement number 3 is thus equivalent to imposing (17) for all composites.

The family of approximate poly-inclusion strain concentrators

$$\hat{\underline{E}} = f(\alpha)\ \underline{E} + g(\alpha)\ \underline{I} \tag{18}$$

is now introduced. Here f(.) and g(.) are arbitrary functions of the fiber concentration. The effective stiffness tensor, associated with the general form (18) via eq. (11), may be expressed as

$$\underline{C} = \underline{C}^m + \alpha \langle [(\underline{C}^f - \underline{C}^m)^{-1} + f(\alpha)\ \underline{E}\ (\underline{C}^m)^{-1} + g(\alpha)\ (\underline{C}^m)^{-1}]^{-1} \rangle. \tag{19}$$

All $\hat{\underline{E}}$ of the form (18) are in compliance with requirement 1, since the contraction $\underline{E}\ (\underline{C}^m)^{-1}$, also known as the 'polarization tensor', is always symmetric (Walpole, 1981). The limit conditions, requirements 2 and 3 - equation (17) - are satisfied if and only if

$$\lim_{\alpha \to 0} f(\alpha) = 1, \quad \lim_{\alpha \to 1} f(\alpha) = 0, \quad \lim_{\alpha \to 0} g(\alpha) = 0, \quad \lim_{\alpha \to 1} g(\alpha) = 0 \tag{20}$$

The simplest concentrator that complies with requirements 1-3 is

thus

$$\hat{\underline{E}} = (1 - \alpha)\underline{E}. \tag{21}$$

which is fully acceptable, for biphase composites with any second-phase geometry, anisotropy, concentration, and orientation distribution, if the associated moduli are in compliance with the appropriate bounds.

The family (18) comprises the classical homogenization schemes. In particular, it may be concluded from (12) that the special case $f = g \equiv 0$ corresponds to Voigt's approach, while $f \equiv 1$, $g \equiv 0$, corresponds to Eshelby's. Voigt's method violates $(20)_1$, and thus requirement 2, while Eshelby's violates (17), and thus requirement 3.

Given (5) and (12), the assumption of Mori-Tanaka may be expressed as

$$\hat{\underline{E}} = \hat{\underline{E}}^{MT} \equiv (1 - \alpha)\underline{E} + \alpha\,(\langle\underline{T}\rangle\,\underline{T}^{-1} - \underline{I}) \tag{22}$$

after some tensorial algebra. By enforcing equation (17) on (22), it is concluded that the the term $\langle\underline{T}\rangle\,\underline{T}^{-1} - \underline{I}$ must identically vanish, in order to avoid unphysical predictions at the unitary second-phase concentration limit. Since, in general, $\underline{T}$ differs from $\langle\underline{T}\rangle$, it is concluded that the scheme of Mori-Tanaka is not acceptable for composites with arbitrary constitution.

Under special circumstances, the Mori-Tanaka scheme does yield a matrix-independent effective stiffness at the unitary concentration limit. In particular, this property is satisfied for biphase composites

with isotropic phases, and for isotropic-matrix biphase composites with perfectly aligned inhomogeneities (Ferrari, 1991). For the latter composite type, an immediate proof is obtained by noting that, in conditions of perfect alignment, the orientation averagings may be dropped, and (22) reduces to (21), which ensures acceptability at the unitary concentration limit.

In the form (21), the Mori-Tanaka assumption may be interpreted as the α-linear interpolation that satisfies the dilute ($\hat{\underline{E}} = \hat{\underline{E}}$) and unitary concentration ($\hat{\underline{E}} = 0$) limits for the eigenstraining poly-inclusion problem under fixed boundary conditions. When not reducible to the form (27), the Mori-Tanaka theory is not applicable, as shown above.

Returning to the general case, it is now recalled that any stiffness of the form (19) is admissible, provided (20) is satified and the relative moduli comply with the appropriate variational bounds. It is not possible to obtain further general restrictions on f(.) and g(.), based on such bounds, as the general optimal bounds on all effective moduli, in terms of the second-phase geometry, concentration, orientation distribution, and anisotropic moduli, are not explicitly available. Thus, a special case of the theory is considered next.

4. CASE STUDIES

For a void second phase, equation (19) specializes to

$$\underline{C} = \underline{C}^{m} \{ \underline{I} + \alpha \langle [f(\alpha)\ \underline{E} + (g(\alpha) - 1)\ \underline{I}\ ]^{-1} \rangle \} \qquad (23)$$

For isotropically distributed cavities in an isotropic matrix, the

effective elastic response is isotropic. In terms of the matrix properties and the void concentration, the optimal bounds on the effective bulk and shear moduli k and μ for this case are those obtained by Hashin and Shtrikman (1963):

$$0 \leq \frac{k}{km} \leq \frac{4(1-\alpha)}{4+3\alpha x}, \quad 0 \leq \frac{\mu}{\mu m} \leq \frac{(1-\alpha)(8+9x)}{8+9x+6\alpha(x+2)} \tag{24}$$

Here, x denotes the matrix bulk-to-shear modulus ratio.

The normalized effective moduli corresponding to (23) are

$$\frac{k}{km} = \frac{(\alpha+h)(3x+4)+3fx}{F1}, \quad \frac{\mu}{\mu m} = \frac{5(\alpha+h)(3x+4)+6f(x+2)}{F2} \tag{25}$$

with the definitions

$$h \equiv g - 1 \; ; \quad F1 \equiv h\,(3x+4) + 3fx \; ; \; F2 \equiv 5h\,(3x+4) + 6f\,(x+2) \tag{26}$$

for the case of spherical voids. Equations (25-26) are conveniently obtained from (23) by the symbolic computing methods introduced in (Ferrari & Marzari, 1992).

Combining (24-26), and simplfying sign definite terms, the bounds on f(.) and h(.) corresponding to the upper Hashin-Shtrikman bounds may be expressed as

$$\frac{k}{km} + \frac{1-\alpha}{F1} \leq 0, \quad \frac{\mu}{\mu m} + \frac{(1-\alpha)(8+9x)}{12\,F2} \leq 0 \tag{27}$$

In view of the positivity of the normalized effective moduli and of the numerators in (27), it follows that F1 and F2 are negative quantities. With this, the bounds may be put in the form

$$3x\ (1 - \alpha) \leq (3x + 4)g + 3fx \leq (1 - \alpha)\ (3x + 4) \tag{28}$$

$$6(1 - \alpha)\ (x + 2) \leq 5(3x + 4)\ g + 6f(x + 2) \leq 5(1 - \alpha)\ (3x + 4) \tag{29}$$

Elementary consideration show that, for

$$(3x - 4)\ f(\alpha) \leq 0 \tag{30}$$

the bound $(28)_2$ is redundant. Otherwise, $(29)_2$ is. Similarly, $(28)_1$ is redundant for

$$(3x - 4)\ g(\alpha) \leq 0 \tag{31}$$

while otherwise $(29)_1$ is. Thus, under the assumption that both f(.) and g(.) be positive definite, the bounds reduce to (28) for $x \geq 4/3$, and to (29) otherwise.

Further assuming that $g(\alpha)$ be identically zero - as done in the Voigt, Eshelby, and Mori-Tanaka theories - the bounds reduce to

$$(1 - \alpha) \leq f(\alpha) \leq (1 - \alpha)\ U\ (x) \tag{32}$$

where

$$U(x) = \frac{3x + 4}{3x} \qquad x \geq 4/3$$

(33)

$$U(x) = \frac{5\,(3x + 4)}{6\,(x + 2)} \qquad x \leq 4/3$$

The region of admissibility corresponding to (32) is shown in Figure 1. There, the gap between the upper and the lower bounds is seen to be a decreasing function of α, for a given material, and to be maximal at $\alpha = 0$, i.e. at a concentration for which the moduli are exactly predicted by (23). Thus, the uncertainty on f(.) and g(.) does not transfer to the effective moduli, in this limit and, arguably, in all sufficiently dilute conditions.

Figure 2 shows that the maximum bound gap at fixed concentration peaks for x=4/3, and then asymptotically tends to zero for increasing values of x.

From (32) it follows that Voigt's assumption $f(.) \equiv 0$ is not admissible for any concentration levels, while the dilute approximation $f(.) \equiv 1$ does not violate the bounds if and only if

$$\alpha \leq \frac{9x + 8}{5(3x + 4)} \qquad x \leq 4/3$$

(34)

$$\alpha \leq \frac{4}{3} \qquad x \geq 4/3.$$

$$3x + 4$$

To visualize: For $x = 3$, representing a high-modulus ceramic, (34) shows that Eshelby's homogenization scheme violates the variational bounds for α larger than 31 %.

The Mori-Tanaka approach, in the context of the present case study, corresponds to $f(\alpha) = 1 - \alpha$. Thus, the bound $(32)_2$ is identically satisfied at all volume fractions and for all materials, and the predictions actually coincide with the bound $(32)_1$.

5. DISCUSSION - CONCLUSIONS

In Section 2, the theory of homogenization was reformulated in terms of the poly-inclusion strain concentrator $\hat{\underline{E}}$. The admissibility criteria, postulated in the introduction, were then re-established in this context, and the family (18) of poly-inclusion strain concentrators was introduced. Any member of this family, for which restrictions (20) hold, is fully admissible, once the appropriate variational bounds on the associated moduli (19) are verified.

In this sense, homogenization based on any of the admissible concentrators of the form (18) is an improvement over all of the existing effective medium theories, since all of these violate one or more of the stated admissibility conditions. The use of (18) is essential especially for composites with a non-dilute concentration of non-aligned or anisotropic inhomogeneities, since none of the 'classic' homogenizations schemes is applicable in such cases.

The homogenization approach based on (18) with $g(.) \equiv 0$ permits an efficient use of the variational bounds, since the bounds on each effective modulus result in a restriction on the single function $f(.)$.

Expressing the effective moduli in terms of a single admissible f(.) also simplifies the experimental determination of the full elastic response, as f(.) may be obtained from easily realizable tensile tests, and then used to predict all other moduli.

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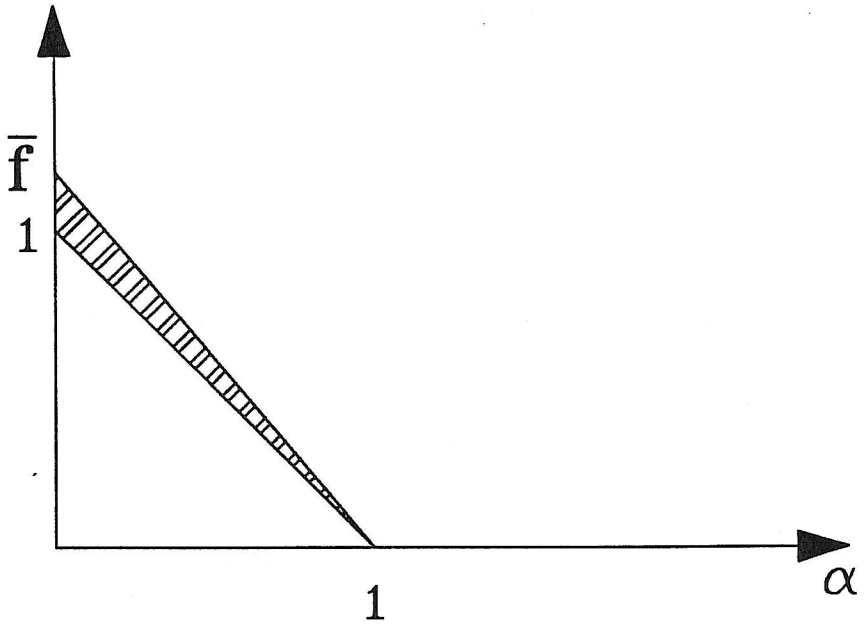

FIG. 1 Domain of admissibility of the function f for g=0. f(.) and g(.) are defined in eq.(18). $\bar{f}=\frac{5(3x+4)}{6(x+2)}$ for $x\leqslant 4/3$, $\bar{f}=\frac{(3x+4)}{3x}$ for $x\geqslant 4/3$.

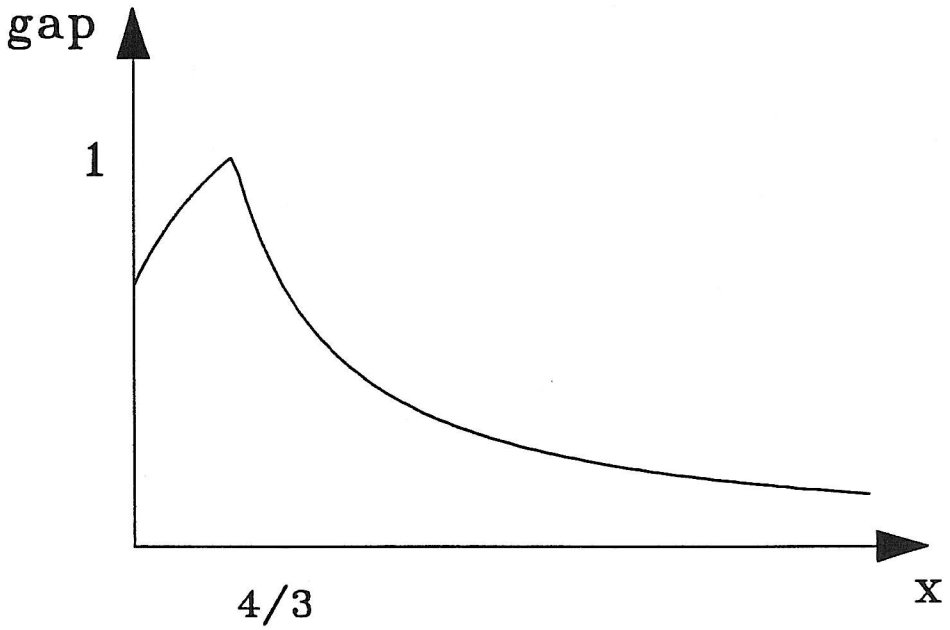

FIG. 2 Maximum gap between bounds as a function of x.