

OPTIMAL BOUNDS ON DISPERSION COEFFICIENT IN ONE-DIMENSIONAL PERIODIC MEDIA

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In this paper, we consider the macroscopic quantity, namely the dispersion tensor associated with a periodic structure in one dimension (see Refs. 5 and 7). We describe the set in which this quantity lies, as the microstructure varies preserving the volume fraction.

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1. Introduction

This work is about macroscopic behavior of fine periodic structures with small period denoted by ε . It is well-known that (see Ref. 3) the homogenization of these structures leads to the first macroscopic quantity, namely the homogenized matrix q

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associated with the periodic structure. We will recall in Sec. 2 the definition of the homogenization problem and the formula for q . It is also known (see Ref. 8) that the spectral approach to the homogenization problem using Bloch waves naturally leads to other macroscopic quantities apart from q . One such quantity is what was called the dispersion tensor d in Refs. 5 and 7. Its definition is recalled in Sec. 2. While q arises in the homogenization of elliptic problems in periodic structures (see Ref. 3), it was noted in Ref. 5 that both (q, d) are required in hyperbolic problems describing propagation of short acoustic waves in such structures. This paper focuses on certain properties of the tensor d .

Inside the class of periodic media, let us consider those with two phases $\{\alpha_0, \alpha_1\}$ with a given volume fraction γ . The arrangement of the phases inside the domain is what constitutes a microstructure. In general, both (q, d) depend on the microstructure in a fairly complicated manner. It is extraordinary to know that q does not depend on the microstructure in one space dimension. (We will recall the relevant formula (2.5) below.) However, in higher dimension, q does vary with the microstructure and a celebrated theorem of Murat and Tartar¹⁰ describes its variation. The discovery in this paper is that the behavior of d even in one space dimension is complicated and it varies with the microstructure as does q in higher dimension. The purpose of this work is to study this dependence and point out the difference in behavior between q and d .

Motivated by applications, let us now consider general optimization problems involving microstructures. It is well-known that a solution does not exist in general and a relaxation procedure is usually followed to overcome this difficulty. What is needed in the description of the relaxed problem is the precise set which contains all the values of q or d as we vary the microstructure. The theorem of Murat and Tartar which uses compensated compactness theory, states that the set of homogenized matrices q , as microstructure varies, is dense in a convex set K_γ (see Refs. 10 and 1, p. 96). In this paper, we initiate the program of deriving analogous results for the macro quantity d . As a first step, we consider the one-dimensional case here. Higher-dimensional problem is more complicated as it involves new phenomena (cf. Conca et al., article in preparation). Contrary to expectation, d exhibits a continuous variation unlike q , as microstructure varies. More precisely, our result Theorem 3.2 shows that d fills up (not merely dense) a bounded interval $I = I(\alpha_0, \alpha_1, \gamma)$ whose end points depend only on α_0, α_1 , and γ , but otherwise are independent of the microstructure. At this time, it is worth to mention the phenomenon of size effect in composites. Size of the specimen of the material being tested has no effect on q , whereas d exhibits size effect. This was proved in Ref. 7. Roughly speaking, when we introduce a large number of interfaces/defects in the microstructure, d decreases and tends to zero as the number of interfaces becomes large. This property lies at the root cause of the above difference in the behavior between q and d . Our construction in Sec. 5 exploits this property. Yet another difference between q and d is as follows: the sets K_γ put together as γ varies in the interval $(0, 1)$ is a convex region, whereas the union of the intervals $I(\alpha_0, \alpha_1, \gamma)$ as γ varies is not convex.

Anticipating future applications, we compute explicitly the end points of I and characterize corresponding microstructures (Theorem 3.1). For this purpose, we exploit the integral representation of d obtained in Ref. 5. Task of finding end points gives rise to a minimization and maximization problem with microstructures. Relaxation method (Sec. 4.1) guarantees existence of optimizers without altering optimal values. Relaxed solutions correspond to generalized microstructures in general. It turns out that minimizer is unique and is a generalized microstructure. Surprisingly, maximizer corresponds to a classical microstructure. Its uniqueness holds in a certain sense (Sec. 4.3.4). Since relaxed problem involves a convex quadratic functional and convex constraints, minimization problem is straightforward, whereas maximization problem is not. The latter problem is studied in Sec. 4.3. Information is gained about maximizers by deriving first-order optimality conditions (Sec. 4.3.1). This allows us to get a new expression for the maximum value of the functional (Sec. 4.3.2) and leads to computation of its exact value (Sec. 4.3.3). At this point, we have proved that the values of the dispersion coefficient are included in the interval $I = I(\alpha_0, \alpha_1, \gamma)$. To complete our study, in the last step, we prove the reverse inclusion, namely, specific periodic microstructures are constructed to show that all points in the interval I are realized as dispersion coefficients (Sec. 5).

2. Preliminaries

Let us introduce some notations adopted in this work. We denote by Y the reference cell $(0, 2\pi)$ and for any real number $\gamma \in [0, 1]$, we consider measurable subsets T of Y such that

$$\frac{|T|}{|Y|} = \gamma.$$

We consider the operator

$$A \stackrel{\text{def}}{=} -\frac{d}{dy} \left(\alpha(y) \frac{d}{dy} \right), \quad y \in \mathbb{R},$$

where the coefficient $\alpha \in L^\infty_\#(Y)$, i.e. $\alpha = \alpha(y)$ is a Y -periodic bounded measurable function defined on \mathbb{R} , and in the reference cell is given by

$$\alpha(y) = \alpha_0 \chi_{T^c}(y) + \alpha_1 \chi_T(y), \quad y \in Y,$$

with $\alpha_0, \alpha_1 > 0, \alpha_0 \neq \alpha_1$. If α_0 and α_1 are equal, the medium will be homogeneous and there is nothing to do. Here $\chi_T(y)$ denotes the characteristic function of T . For each $\varepsilon > 0$, we consider also the εY -periodic operator A^ε defined by

$$A^\varepsilon \stackrel{\text{def}}{=} -\frac{d}{dx} \left(\alpha^\varepsilon(x) \frac{d}{dx} \right) \quad \text{with} \quad \alpha^\varepsilon(x) \stackrel{\text{def}}{=} \alpha\left(\frac{x}{\varepsilon}\right), \quad x \in \mathbb{R}.$$

In homogenization theory, it is usual to refer to x and y the slow and the fast variables, respectively. They are related by $y = \frac{x}{\varepsilon}$.

Macro quantities (q, d) are defined in terms of Bloch waves ψ associated with the operator A which we introduce now. Let us consider the following spectral problem parametrized by $\eta \in \mathbb{R}$: find $\lambda = \lambda(\eta) \in \mathbb{R}$ and $\psi = \psi(y; \eta)$ (not identically zero) such that

$$\begin{cases} A\psi(\cdot; \eta) = \lambda(\eta)\psi(\cdot; \eta) \text{ in } \mathbb{R}, & \psi(\cdot; \eta) \text{ is } (\eta; Y)\text{-periodic, i.e.} \\ \psi(y + 2\pi m; \eta) = e^{2\pi im\eta}\psi(y; \eta) & \forall m \in \mathbb{Z}, \quad y \in \mathbb{R}. \end{cases} \tag{2.1}$$

Next, by the Floquet theory, we define $\phi(y; \eta) = e^{-iy\eta}\psi(y; \eta)$ and (2.1) can be rewritten in terms of ϕ as follows:

$$A(\eta)\phi = \lambda\phi \text{ in } \mathbb{R}, \quad \phi \text{ is } Y\text{-periodic.} \tag{2.2}$$

Here, the operator $A(\eta)$ is called the translated operator and is defined by

$$A(\eta) = e^{-iy\eta} A e^{iy\eta}.$$

It is well-known (see Refs. 3 and 6) that for each $\eta \in Y' = [-\frac{1}{2}, \frac{1}{2})$, the above spectral problem (2.2) admits a discrete sequence of eigenvalues $\lambda_m(\eta)$ and their eigenfunctions $\phi_m(y; \eta)$ (referred to as *Bloch waves*) enable us to describe the spectral resolution of A (as an unbounded self-adjoint operator in $L^2(\mathbb{R})$) in the orthogonal basis $\{e^{iy\eta}\phi_m(y; \eta) : m \geq 1, \eta \in Y'\}$.

Let us introduce Bloch waves at the ε -scale:

$$\lambda_m^\varepsilon(\xi) = \varepsilon^{-2}\lambda_m(\eta), \quad \phi_m^\varepsilon(x; \xi) = \phi_m(y; \eta), \quad \psi_m^\varepsilon(x; \xi) = \psi_m(y; \eta),$$

where the variables (x, ξ) and (y, η) are related by $y = \frac{x}{\varepsilon}$ and $\eta = \varepsilon\xi$. Observe that $\phi_m^\varepsilon(x; \xi)$ is εY -periodic (with respect to x) and $\varepsilon^{-1}Y'$ -periodic with respect to ξ . In the same manner, $\psi_m^\varepsilon(\cdot; \xi)$ is $(\xi; \varepsilon Y)$ -periodic because of the relation $\psi_m^\varepsilon(x; \xi) = e^{ix\xi}\phi_m^\varepsilon(x; \xi)$. Note that the dual cell at ε -scale is $\varepsilon^{-1}Y'$ and hence we take ξ to vary in $\varepsilon^{-1}Y'$.

We consider a sequence $\{u^\varepsilon\}$ bounded in $H^1(\mathbb{R})$ and $f \in L^2(\mathbb{R})$ satisfying

$$A^\varepsilon u^\varepsilon = f \text{ in } \mathbb{R}. \tag{2.3}$$

We assume that $u^\varepsilon \rightharpoonup u$ weakly in $H^1(\mathbb{R})$. The homogenization problem consists of passing to the limit, as $\varepsilon \rightarrow 0$, in the previous equation and obtain the equation satisfied by u , namely,

$$Qu \stackrel{\text{def}}{=} -q \frac{d^2 u}{dx^2} = f \text{ in } \mathbb{R}, \tag{2.4}$$

where q is a constant known as the homogenized coefficient (see Ref. 3).

Simple relation linking q with Bloch waves is the following: $q = \frac{1}{2}\lambda_1^{(2)}(0)$ (see Ref. 4). At this point, it is appropriate to recall that derivatives of the first eigenvalue and eigenfunction at $\eta = 0$ exist thanks to the regularity property established in Ref. 8. In fact, we know that there exists $\delta_0 > 0$ such that the first eigenvalue $\lambda_1(\eta)$ is an analytic function on $B_{\delta_0} = \{\eta : |\eta| < \delta_0\}$, and there is a choice of the first

eigenvector $\phi_1(y; \eta)$ satisfying

$$\eta \mapsto \phi_1(\cdot; \eta) \in H^1_{\#}(Y) \text{ is analytic on } B_{\delta_0}, \quad \phi_1(y; 0) = |Y|^{-1/2} = \frac{1}{(2\pi)^{N/2}}.$$

To see how d arises, let us consider wave propagation problem in the periodic structure governed by the operator $\partial_{tt} + A^\varepsilon$ with appropriate initial conditions. If we consider short waves of low energy with wave number satisfying $\varepsilon^2|\xi|^4 = O(1)$ and $\varepsilon^4|\xi|^6 = o(1)$ then a simplified description is obtained with the operator $\partial_{tt} + Q + \varepsilon^2 D$, where D is the fourth-order operator whose symbol is $\frac{1}{4!}\lambda_1^{(4)}(0)\xi^4$. This was noted in Ref. 5. Important tensor $d = \frac{1}{4!}\lambda_1^{(4)}(0)$, which captures dispersive effects on such waves, represents a corrector to the periodic medium. It was studied in Ref. 5 and in particular, a physical space representation for it was obtained. We recall it, in the one-dimensional case in the result below:

Proposition 2.1. *We have the relations*

$$\lambda_1(0) = 0, \quad \lambda_1^{(1)}(0) = 0, \quad \frac{1}{2!}\lambda_1^{(2)}(0) = q, \quad \frac{1}{3!}\lambda_1^{(3)}(0) = 0, \quad \frac{1}{4!}\lambda_1^{(4)}(0) = d,$$

where q can be explicitly expressed

$$\frac{1}{q} = \frac{\gamma}{\alpha_1} + \frac{1 - \gamma}{\alpha_0}. \tag{2.5}$$

Moreover, the dispersion coefficient d admits the following representation:

$$d = -\frac{q}{|Y|} \int_Y (X_{(T)})^2, \tag{2.6}$$

with test function $X_{(T)}$ defined by the following cell problem:

$$\begin{cases} -\frac{dX_{(T)}}{dy} = 1 - q\left(\frac{\chi_T}{\alpha_1} + \frac{1 - \chi_T}{\alpha_0}\right) & \text{in } \mathbb{R}, \\ X_{(T)} \in H^1_{\#}(Y), \quad \frac{1}{|Y|} \int_Y X_{(T)}(y) dy = 0. \end{cases} \tag{2.7}$$

Remark 2.1. The formula (2.5) shows that q does not depend on the microstructure. Moreover, the following useful identities hold:

$$\frac{1}{q} - \frac{1}{\alpha_0} = \gamma\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right), \tag{2.8}$$

$$\frac{1}{\alpha_1} - \frac{1}{q} = (1 - \gamma)\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right). \tag{2.9}$$

On the other hand, formulae (2.6) and (2.7) show explicitly how the dispersion coefficient d depends on the microstructure through the characteristic function χ_T .

3. Main Results

The purpose of this section is to present our main results concerning the set in which the dispersion coefficient d lies, as the microstructure varies preserving the volume proportion γ . Let us first observe that if $\gamma \in \{0, 1\}$, the dispersion coefficient d is equal to 0. For this reason, we take $\gamma \in (0, 1)$ in the sequel.

We introduce some notations. Let us denote by $\text{Char}(Y)$ the set of all characteristic functions of measurable subsets of Y , i.e.

$$\text{Char}(Y) = \{\chi : Y \rightarrow \{0, 1\} \text{ measurable}\}.$$

Moreover, for any $\chi \in \text{Char}(Y)$ we denote by $T(\chi) = \{y \in Y : \chi(y) = 1\}$. For a given $\gamma \in (0, 1)$, let us consider the set \mathcal{C}_γ of classical microstructures defined by

$$\mathcal{C}_\gamma = \{\chi \in \text{Char}(Y) : |T(\chi)| = \gamma|Y|\}$$

and for any $\chi \in \text{Char}(Y)$, we define the functional $J_0(\chi)$ as follows

$$J_0 : \text{Char}(Y) \rightarrow \mathbb{R}$$

$$\chi \mapsto J_0(\chi) \stackrel{\text{def}}{=} \frac{1}{|Y|} \int_Y (X_{T(\chi)})^2,$$

where $X_{T(\chi)}$ is the solution of Eq. (2.7).

Using these notations, the dispersion coefficient can be rewritten as follows

$$d(\chi_T) = -qJ_0(\chi_T)$$

and therefore, it is obvious that

$$-q \sup_{\chi \in \mathcal{C}_\gamma} J_0(\chi) \leq d(\chi_T) \leq -q \inf_{\chi \in \mathcal{C}_\gamma} J_0(\chi) \quad \forall \chi_T \in \mathcal{C}_\gamma.$$

In order to find the exact values of the previous supremum and infimum, we proceed to the relaxation of the minimization and maximization problems. To do this, for any $\gamma \in (0, 1)$, let us consider the set \mathcal{D}_γ of generalized microstructures defined by

$$\mathcal{D}_\gamma = \{\theta \in L^\infty_\#(Y; [0, 1]) : \mathfrak{m}(\theta) = \gamma\},$$

where $\mathfrak{m}(f)$ denotes the average of the function f over Y , that is,

$$\mathfrak{m}(f) = \frac{1}{|Y|} \int_Y f(y) dy.$$

Recall that $\theta(y)$ represents local volume proportion of the material α_1 at y in the generalized microstructure. Moreover, we define the extension of the functional J_0 over $L^\infty_\#(Y; [0, 1])$, denoted by $J(\theta)$, as follows

$$J : L^\infty_\#(Y; [0, 1]) \rightarrow \mathbb{R}$$

$$\theta \mapsto J(\theta) \stackrel{\text{def}}{=} \mathfrak{m}((X_\theta)^2),$$

where X_θ is the solution of the following relaxed version of the problem (2.7):

$$\begin{cases} -\frac{dX_\theta}{dy} = 1 - q(\mathcal{M}(\theta))\left(\frac{\theta}{\alpha_1} + \frac{1-\theta}{\alpha_0}\right) & \text{in } \mathbb{R}, \\ X_\theta \in H^1_{\#}(Y), \quad \mathcal{M}(X_\theta) = 0 \end{cases} \tag{3.1}$$

and $q(\cdot)$ is defined by

$$\frac{1}{q(\tau)} = \frac{\tau}{\alpha_1} + \frac{1-\tau}{\alpha_0}. \tag{3.2}$$

Remark 3.1. Let us observe that

$$q(\mathcal{M}(\theta)) = q(\gamma) = q \quad \forall \theta \in \mathcal{D}_\gamma,$$

where q is defined in (2.5).

Thus the dispersion coefficient d , which is *a priori* defined for microstructures in \mathcal{C}_γ , can be extended to generalized microstructures in \mathcal{D}_γ .

We now state our first main result, which computes the optimal lower and upper bounds of $d(\chi_T)$, as the microstructure χ_T varies such that $|T| = \gamma|Y|$.

Theorem 3.1. *For any $\gamma \in (0, 1)$, we have that*

$$\inf_{\chi \in \mathcal{C}_\gamma} J_0(\chi) = \min_{\theta \in \mathcal{D}_\gamma} J(\theta), \quad \sup_{\chi \in \mathcal{C}_\gamma} J_0(\chi) = \max_{\theta \in \mathcal{D}_\gamma} J(\theta), \tag{3.3}$$

$$\min_{\theta \in \mathcal{D}_\gamma} J(\theta) = 0, \tag{3.4}$$

$$\max_{\theta \in \mathcal{D}_\gamma} J(\theta) = \frac{1}{12} q^2 \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2. \tag{3.5}$$

Moreover, there exists a unique generalized microstructure $\theta^*_{\min} \in \mathcal{D}_\gamma$ minimizer for the problem (3.4). There is a classical microstructure $\theta^*_{\max} \in \mathcal{C}_\gamma$ which is maximizer for the problem (3.5). The maximizer is also unique up to a translation.

With regard to the above result, let us note that the functional J is convex and quadratic. Further, we have convex and linear constraints in our problem. Minimization is thus straightforward; however maximization is not. As a direct consequence of Theorem 3.1 we obtain the following result:

Corollary 3.1. *For any $\gamma \in (0, 1)$, the following inclusion holds:*

$$\{d(\chi) : \chi \in \mathcal{C}_\gamma\} \subseteq \left[-\frac{1}{12} q^3 \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2, 0\right).$$

For $\gamma \in \{0, 1\}$, we have $d(\chi) = 0 \quad \forall \chi \in \mathcal{C}_\gamma$.

Theorem 3.1 and its Corollary 3.1 give the optimal bounds on the dispersion coefficient $d(\chi)$ for all microstructures $\chi \in \mathcal{C}_\gamma$. In the sequel, we go further and we

prove that for any real number $D_0 \in [-\frac{1}{12}q^3\gamma^2(1-\gamma)^2|Y|^2(\frac{1}{\alpha_1} - \frac{1}{\alpha_0})^2, 0)$, there exists a composite material defined by a characteristic function $\chi \in \mathcal{C}_\gamma$ such that $d(\chi) = D_0$. That is, the dispersion coefficient fills up the above interval. This second main result is stated in the following theorem:

Theorem 3.2. *For any $\gamma \in (0, 1)$, the following equality holds:*

$$\{d(\chi) : \chi \in \mathcal{C}_\gamma\} = \left[-\frac{1}{12}q^3\gamma^2(1-\gamma)^2|Y|^2\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2, 0 \right).$$

Here we see a behavior of d different from that of homogenized matrix in multi-dimension. As periodic microstructure varies, the set of homogenized matrices is dense but does not fill up the region K_γ .

Remark 3.2. Let us consider the dispersion coefficient as a function in terms of the data α_0, α_1 , and γ and let us denote it by $d(\alpha_0, \alpha_1, \gamma, \chi_T)$. Using the state equation (2.7) and the definition of q , we have

$$d(\alpha_0, \alpha_1, \gamma, \chi_T) = d(\alpha_1, \alpha_0, 1 - \gamma, \chi_{T^c}).$$

If we denote by $d_{\min}(\alpha_0, \alpha_1, \gamma) = \inf_{\chi_T \in \mathcal{C}_\gamma} d(\alpha_0, \alpha_1, \gamma, \chi_T)$, using the previous identity we obtain

$$d_{\min}(\alpha_0, \alpha_1, \gamma) = d_{\min}(\alpha_1, \alpha_0, 1 - \gamma).$$

The bounds that are established in Theorem 3.1 fulfill the above symmetry.

4. Proof of First Main Result

In this section, we prove Theorem 3.1 in several steps.

4.1. Relaxation

When dealing with minimization and maximization problems involving microstructures, of the form

$$\inf_{\chi \in \mathcal{C}_\gamma} J_0(\chi) \quad \text{and} \quad \sup_{\chi \in \mathcal{C}_\gamma} J_0(\chi),$$

it is known that they do not in general admit solutions within the class of classical microstructures. To overcome this, the proposed way is relaxation which amounts to passage from classical to generalized microstructures. The purpose of this subsection is to relax the above minimization and maximization problems and prove the identities (3.3) of Theorem 3.1. Thus relaxation procedure does not alter the optimal values, a fact well-known in the literature. For the sake of completeness, we briefly recall the arguments.

We first remark that the set \mathcal{C}_γ is dense in \mathcal{D}_γ and \mathcal{D}_γ is a compact subset of $L^\infty_\#(Y)$, with the weak* topology of $L^\infty(Y)$ (see Proposition 4 and Remark 7 in Ref. 10). Because of this, using Proposition 2 in Ref. 10, it is enough to prove that for

any sequence of characteristic functions $\{\chi_n\} \subset \mathcal{C}_\gamma$ weak* convergent to $\theta \in \mathcal{D}_\gamma$ in $L^\infty(Y)$, we have

$$J_0(\chi_n) \rightarrow J(\theta),$$

i.e. the functional J is weak* continuous.

Let us verify that this property holds. In fact, we consider a sequence of characteristic functions $\{\chi_n\} \subset \mathcal{C}_\gamma$ that weak* converges to $\theta \in \mathcal{D}_\gamma$ in $L^\infty(Y)$. Using Eq. (2.7), we deduce that the sequence $\{X_{(T(\chi_n))}\}$ is bounded in $W^{1,\infty}(Y)$, and so there exists $X \in H^1_\#(Y)$ such that

$$X_{(T(\chi_n))} \rightharpoonup X \text{ weakly in } H^1_\#(Y).$$

Hence, due to Rellich's theorem we get

$$X_{(T(\chi_n))} \rightarrow X \text{ strongly in } L^2_\#(Y).$$

With this strong convergence, we obtain

$$J_0(\chi_n) \rightarrow \mathcal{M}(X^2).$$

Finally, passing to the limit in Eq. (2.7) written for $T(\chi_n)$, it follows that the limit X satisfies Eq. (3.1) because $q = q(\mathcal{M}(\theta))$. Therefore, $\mathcal{M}(X^2) = J(\theta)$ and we conclude that the equalities (3.3) hold.

4.2. Minimization problem on \mathcal{D}_γ

In this subsection, we prove the equality (3.4) of Theorem 3.1. First of all, it is clear that for all $\theta \in \mathcal{D}_\gamma$ we have $J(\theta) \geq 0$. Now, let us prove that there exists $\theta^*_{\min} \in \mathcal{D}_\gamma$ such that $J(\theta^*_{\min}) = 0$, i.e. $X_{\theta^*_{\min}} = 0$. More precisely, using (3.1), we are looking for $\theta^*_{\min} \in \mathcal{D}_\gamma$ such that

$$q\left(\frac{\theta^*_{\min}(y)}{\alpha_1} + \frac{1 - \theta^*_{\min}(y)}{\alpha_0}\right) = 1,$$

that is,

$$\theta^*_{\min}(y) = \frac{\frac{1}{q} - \frac{1}{\alpha_0}}{\frac{1}{\alpha_1} - \frac{1}{\alpha_0}}.$$

Since (2.8) holds, we find

$$\theta^*_{\min}(\cdot) \equiv \gamma.$$

Thus, the minimizer is unique and it is a generalized microstructure given by the rule that local volume proportion of the α_1 -material is constant throughout the microstructure.

4.3. Maximization problem on \mathcal{D}_γ

In this subsection, we prove the equality (3.5) of Theorem 3.1. We divide the proof in several steps.

4.3.1. *Optimality condition*

First of all, since \mathcal{D}_γ is compact with respect to weak* topology on $L^\infty(Y)$ and J is continuous (as seen above), maximizers for J over \mathcal{D}_γ do exist. To get information on them, since our problem has the structure of an optimal control problem with control constraints, we are inspired by the existing treatment of such problems. However, one should note that our problem is ill-posed in the sense that we are dealing with maximization (instead of minimization) of a quadratic, convex functional over a convex set with an equality constraint. It is then natural to dualize the equality constraint $\mathcal{m}(\theta) = \gamma$ by means of a Lagrange multiplier λ and introduce a Lagrangian $L(\theta, \lambda)$ as follows

$$L(\theta, \lambda) = J(\theta) + \lambda(\mathcal{m}(\theta) - \gamma) \quad \forall \theta \in L^\infty_\#(Y; [0, 1]), \quad \forall \lambda \in \mathbb{R}. \tag{4.1}$$

Generally, optimality condition at a maximizer is expressed in terms of derivative of L at maximizer. As a first step, we proceed to compute the derivative via the introduction of adjoint state.

For a given $\theta_0 \in \mathcal{D}_\gamma$, let us compute the derivative $D_\theta L(\theta_0, \lambda)(\theta - \theta_0)$. Using the definition (4.1), we get

$$D_\theta L(\theta_0, \lambda)(\theta - \theta_0) = \mathcal{m}(2X_{\theta_0} D_\theta X_{\theta_0}(\theta - \theta_0)) + \lambda \mathcal{m}(\theta - \theta_0). \tag{4.2}$$

In order to compute the derivative of X_θ , let us introduce the following notation

$$\delta X_\theta = D_\theta X_\theta(\theta_0)(\theta - \theta_0).$$

We differentiate Eqs. (3.1) and (3.2) with respect to θ and we use Remark 3.1. Then, we get

$$\begin{cases} -\frac{d}{dy}(\delta X_\theta) = -q'(\mathcal{m}(\theta_0))\mathcal{m}(\theta - \theta_0)\left(\frac{\theta_0}{\alpha_1} + \frac{1 - \theta_0}{\alpha_0}\right) \\ \qquad \qquad \qquad - q\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)(\theta - \theta_0) \quad \text{in } \mathbb{R}, \\ \delta X_\theta \in H^1_\#(Y), \quad \mathcal{m}(\delta X_\theta) = 0, \end{cases} \tag{4.3}$$

with

$$q'(\mathcal{m}(\theta_0)) = -q^2\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right). \tag{4.4}$$

Now, to compute the term $\mathcal{m}(2X_{\theta_0} \delta X_\theta)$ appearing in the right-hand side of the identity (4.2), we introduce the following adjoint state equation: for all $\theta \in L^\infty_\#(Y; [0, 1])$, let P_θ be the solution of the problem

$$\begin{cases} -\frac{dP_\theta}{dy} = 2q\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)X_\theta \quad \text{in } \mathbb{R}, \\ P_\theta \in H^1_\#(Y), \quad \mathcal{m}(P_\theta) = 0. \end{cases} \tag{4.5}$$

Using this adjoint state equation with $\theta = \theta_0$ and integrating by parts, we obtain that

$$\mathfrak{m}(2X_{\theta_0} \delta X_\theta) = -\mathfrak{m} \left(\frac{dP_{\theta_0}}{dy} \frac{1}{q(\frac{1}{\alpha_1} - \frac{1}{\alpha_0})} \delta X_\theta \right) = \mathfrak{m} \left(\frac{P_{\theta_0}}{q(\frac{1}{\alpha_1} - \frac{1}{\alpha_0})} \frac{d}{dy} (\delta X_\theta) \right).$$

Then, due to Eqs. (4.3) and (4.4), it follows that

$$\mathfrak{m}(2X_{\theta_0} \delta X_\theta) = \mathfrak{m} \left(P_{\theta_0}(\theta - \theta_0) - q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) P_{\theta_0} \theta_0 \mathfrak{m}(\theta - \theta_0) \right).$$

Therefore, the identity (4.2) gives that for all $\theta \in L^\infty_{\#}(Y; [0, 1])$ and for all $\lambda \in \mathbb{R}$,

$$D_\theta L(\theta_0, \lambda)(\theta - \theta_0) = \mathfrak{m}(P_{\theta_0}(\theta - \theta_0)) + \left[\lambda - q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{m}(P_{\theta_0} \theta_0) \right] \mathfrak{m}(\theta - \theta_0). \tag{4.6}$$

Having computed the derivative, let us now prove the following optimality condition:

Proposition 4.1. *For each $\theta^* \in \mathcal{D}_\gamma$ such that $J(\theta^*) = \max_{\theta \in \mathcal{D}_\gamma} J(\theta)$, we have:*

(i) *There exists $\lambda^* \in \mathbb{R}$ such that*

$$D_\theta L(\theta^*, \lambda^*)(\theta - \theta^*) \leq 0 \quad \forall \theta \in L^\infty_{\#}(Y; [0, 1]). \tag{4.7}$$

(ii) *There exists $p^* \in \mathbb{R}$ such that the following optimality condition holds:*

$$\begin{cases} \theta^* \in [0, 1] & \text{a.e. in } \mathcal{A}(\theta^*, p^*), \\ \theta^* = 1 & \text{a.e. in } \mathcal{B}(\theta^*, p^*), \\ \theta^* = 0 & \text{a.e. in } \mathcal{C}(\theta^*, p^*), \end{cases} \tag{4.8}$$

where the sets $\mathcal{A}(\theta^*, p^*)$, $\mathcal{B}(\theta^*, p^*)$ and $\mathcal{C}(\theta^*, p^*)$ are defined by

$$\mathcal{A}(\theta^*, p^*) = \{y \in \mathbb{R} : P_{\theta^*}(y) = p^*\}, \tag{4.9}$$

$$\mathcal{B}(\theta^*, p^*) = \{y \in \mathbb{R} : P_{\theta^*}(y) > p^*\}, \tag{4.10}$$

$$\mathcal{C}(\theta^*, p^*) = \{y \in \mathbb{R} : P_{\theta^*}(y) < p^*\}. \tag{4.11}$$

Remark 4.1. Point (i) of the above result says that the principle of Lagrange multiplier holds in the present problem. Usually the required Lagrange multiplier λ^* is obtained from a saddle point for L at θ^* . Such a structure is missing here because θ^* is a maximizer for the convex functional J . The proof shows how to get around this difficulty to get λ^* . Point (ii) describes the generalized microstructure defined by the maximizer θ^* in terms of the associated adjoint state. While (i) presents an average property of θ^* , point (ii) which is deduced from (i) gives a pointwise property of θ^* .

Proof. Let us prove (i). Using the identity (4.6), for each $\theta^* \in \mathcal{D}_\gamma$ such that $J(\theta^*) = \max_{\theta \in \mathcal{D}_\gamma} J(\theta)$, we have that for all $\theta \in L^\infty_\#(Y; [0, 1])$ and $\lambda \in \mathbb{R}$,

$$D_\theta L(\theta^*, \lambda)(\theta - \theta^*) = \mathfrak{m}(P_{\theta^*}(\theta - \theta^*)) + \left[\lambda - q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{m}(P_{\theta^*}\theta^*) \right] \mathfrak{m}(\theta - \theta^*). \tag{4.12}$$

In order to estimate the first term of the previous expression, let us introduce the function G defined as follows:

$$G : L^\infty_\#(Y; [0, 1]) \rightarrow \mathbb{R} \\ \theta \mapsto G(\theta) \stackrel{\text{def}}{=} \mathfrak{m}(P_\theta\theta).$$

Since the function $G(\cdot)$ is continuous with respect to L^∞ -weak* topology, there exists $\tilde{\theta}^* \in \mathcal{D}_\gamma$ such that $G(\tilde{\theta}^*) = \max_{\theta \in \mathcal{D}_\gamma} G(\theta)$. Let us consider the Lagrangian $M(\theta, \mu)$ associated with the above maximization problem for $G(\theta)$:

$$M(\theta, \mu) = G(\theta) - \mu \mathfrak{m}(\theta - \gamma) \quad \forall \theta \in L^\infty_\#(Y; [0, 1]), \quad \forall \mu \in \mathbb{R}.$$

There exists $\tilde{\mu}^* \in \mathbb{R}$ such that

$$M(\theta, \tilde{\mu}^*) \leq M(\tilde{\theta}^*, \tilde{\mu}^*) \leq M(\tilde{\theta}^*, \mu) \quad \forall \theta \in L^\infty_\#(Y; [0, 1]), \quad \forall \mu \in \mathbb{R} \tag{4.13}$$

(see Ref. 9, p. 173). It is worth to remark that such a saddle point structure was absent with (J, L) whereas it is available with (G, M) .

Due to the definitions of G and M and the fact that $\tilde{\theta}^* \in \mathcal{D}_\gamma$, the first inequality yields

$$\mathfrak{m}(P_{\theta^*}(\theta - \tilde{\theta}^*)) \leq \tilde{\mu}^* \mathfrak{m}(\theta - \gamma). \tag{4.14}$$

Let us observe that if we consider the particular case $\theta = \tilde{\theta}^*$ in Eq. (4.12), we get

$$D_\theta L(\theta^*, \lambda)(\tilde{\theta}^* - \theta^*) = \mathfrak{m}(P_{\theta^*}(\tilde{\theta}^* - \theta^*)).$$

On the other hand, since $\tilde{\theta}^* \in \mathcal{D}_\gamma$, we have that $D_\theta L(\theta^*, \lambda)(\tilde{\theta}^* - \theta^*) = D_\theta J(\theta^*)(\tilde{\theta}^* - \theta^*)$, and therefore

$$D_\theta J(\theta^*)(\tilde{\theta}^* - \theta^*) = \mathfrak{m}(P_{\theta^*}(\tilde{\theta}^* - \theta^*)). \tag{4.15}$$

Adding and subtracting the function $\tilde{\theta}^*$, the Eq. (4.12) can be rewritten as follows

$$D_\theta L(\theta^*, \lambda)(\theta - \theta^*) = \mathfrak{m}(P_{\theta^*}(\tilde{\theta}^* - \theta^*)) + \mathfrak{m}(P_{\theta^*}(\theta - \tilde{\theta}^*)) + \left[\lambda - q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{m}(P_{\theta^*}\theta^*) \right] \mathfrak{m}(\theta - \theta^*).$$

Then, using the inequality (4.14) and the identity (4.15) in the above relation, we deduce that

$$D_\theta L(\theta^*, \lambda)(\theta - \theta^*) \leq D_\theta J(\theta^*)(\tilde{\theta}^* - \theta^*) + \left[\tilde{\mu}^* + \lambda - q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{M}(P_{\theta^*} \theta^*) \right] \mathfrak{M}(\theta - \theta^*). \tag{4.16}$$

Let us now choose

$$\lambda^* \stackrel{\text{def}}{=} -\tilde{\mu}^* + q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{M}(P_{\theta^*} \theta^*). \tag{4.17}$$

With this choice, (4.16) becomes

$$D_\theta L(\theta^*, \lambda^*)(\theta - \theta^*) \leq D_\theta J(\theta^*)(\tilde{\theta}^* - \theta^*).$$

Hence, the inequality (4.7) is a direct consequence of the fact that the maximum in \mathcal{D}_γ of the functional J is attained in θ^* .

Let us now prove (ii). Using (4.12), the inequality (4.7) yields

$$\int_Y (P_{\theta^*}(y) - p^*)(\theta(y) - \theta^*(y)) dy \leq 0 \quad \forall \theta \in L^\infty_\#(Y; [0, 1]), \tag{4.18}$$

where

$$p^* = -\lambda^* + q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \mathfrak{M}(P_{\theta^*} \theta^*). \tag{4.19}$$

From the integral inequality (4.18), we now deduce some pointwise information on θ^* . In the sequel, we prove that $\theta^* = 1$ almost everywhere in $\mathcal{B}(\theta^*, p^*) \cap Y$. To this end, we define the set

$$E = \{y \in \mathcal{B}(\theta^*, p^*) \cap Y : \theta^*(y) < 1\}$$

and the function

$$\theta_E(y) = \begin{cases} 1 & \text{if } y \in E, \\ \theta^*(y) & \text{if } y \in Y \setminus E. \end{cases}$$

Using this test function in inequality (4.18), we obtain

$$\int_E (P_{\theta^*}(y) - p^*)(1 - \theta^*(y)) dy \leq 0.$$

Since $(P_{\theta^*}(y) - p^*)(1 - \theta^*(y)) > 0$ for all $y \in E$, we deduce that E is a null set and so $\theta^* = 1$ almost everywhere in $\mathcal{B}(\theta^*, p^*) \cap Y$.

Analogously, one can prove $\theta^* = 0$ almost everywhere in $\mathcal{C}(\theta^*, p^*) \cap Y$. Hence, by periodicity we get (4.8) and so proposition is proved. \square

4.3.2. *New expression of J*

Let us denote by Θ_γ the set of all $\theta^* \in \mathcal{D}_\gamma$ where the optimality condition (4.8) holds, that is,

$$\Theta_\gamma = \{\theta^* \in \mathcal{D}_\gamma : \text{there exists } p^* \in \mathbb{R} \text{ such that (4.8) holds}\}. \tag{4.20}$$

Note that maximizers lie in this set.

In the next result, we describe the structure of the sets $\mathcal{A}(\theta^*, p^*)$, $\mathcal{B}(\theta^*, p^*)$, and $\mathcal{C}(\theta^*, p^*)$ defined in (4.9)–(4.11). Here one-dimensional nature of the problem is exploited.

Lemma 4.1. *For any $(\theta^*, p^*) \in \Theta_\gamma \times \mathbb{R}$ such that (4.8) holds, the following properties are true:*

- (i) $\mathcal{A}(\theta^*, p^*) \neq \emptyset$.
- (ii) $\partial\mathcal{B}(\theta^*, p^*) \cup \partial\mathcal{C}(\theta^*, p^*) \subseteq \mathcal{A}(\theta^*, p^*)$.
- (iii) *For a given $y_{\mathcal{A}} \in \mathcal{A}(\theta^*, p^*)$ there exist two collections of disjoint open intervals $\{(a_i, b_i)\}_{i=1}^{N_{\mathcal{B}}}$ and $\{(c_j, d_j)\}_{j=1}^{N_{\mathcal{C}}}$ such that*

$$\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y) = \bigcup_{i=1}^{N_{\mathcal{B}}} (a_i, b_i) \tag{4.21}$$

and

$$\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y) = \bigcup_{j=1}^{N_{\mathcal{C}}} (c_j, d_j), \tag{4.22}$$

where $N_{\mathcal{B}}, N_{\mathcal{C}} \in \mathbb{N} \cup \{+\infty\}$ and $a_i, b_i, c_j, d_j \in \mathcal{A}(\theta^*, p^*)$ for all $i \in \{1, \dots, N_{\mathcal{B}}\}$, $j \in \{1, \dots, N_{\mathcal{C}}\}$. Moreover, we have:

$$\sum_{i=1}^{N_{\mathcal{B}}} (b_i - a_i) \leq \gamma|Y| \tag{4.23}$$

and

$$\sum_{j=1}^{N_{\mathcal{C}}} (d_j - c_j) \leq (1 - \gamma)|Y|. \tag{4.24}$$

Proof. In order to prove (i) we proceed by contradiction and we suppose that $\mathcal{A}(\theta^*, p^*) = \emptyset$. With this, we deduce that $\mathcal{B}(\theta^*, p^*) = \mathbb{R}$ or $\mathcal{C}(\theta^*, p^*) = \mathbb{R}$ because $P_{\theta^*}(\cdot)$ is a continuous function. Hence, we obtain $\mathcal{M}(\theta^*) = 1$ or $\mathcal{M}(\theta^*) = 0$ (see the optimality condition (4.8)), which is a contradiction with the fact that $\mathcal{M}(\theta^*) = \gamma \in (0, 1)$.

Let us now prove (ii). To this end, we first consider an arbitrary $\bar{y} \in \partial\mathcal{B}(\theta^*, p^*)$. Then, there exist $\{x_n\}_{n \in \mathbb{N}} \subseteq \mathcal{B}(\theta^*, p^*)$ and $\{y_n\}_{n \in \mathbb{N}} \subseteq \mathbb{R} \setminus \mathcal{B}(\theta^*, p^*) = \mathcal{A}(\theta^*, p^*) \cup$

$\mathcal{C}(\theta^*, p^*)$ such that

$$x_n \rightarrow \bar{y} \quad \text{and} \quad y_n \rightarrow \bar{y}, \quad \text{as } n \rightarrow \infty.$$

Using the fact that P_{θ^*} is a continuous function, we obtain

$$P_{\theta^*}(x_n) \rightarrow P_{\theta^*}(\bar{y}) \quad \text{and} \quad P_{\theta^*}(y_n) \rightarrow P_{\theta^*}(\bar{y}), \quad \text{as } n \rightarrow \infty. \tag{4.25}$$

On the other hand, using definitions (4.9)–(4.11) of the sets $\mathcal{A}(\theta^*, p^*)$, $\mathcal{B}(\theta^*, p^*)$, and $\mathcal{C}(\theta^*, p^*)$, we get that

$$P_{\theta^*}(x_n) > p^* \quad \text{and} \quad P_{\theta^*}(y_n) \leq p^* \quad \text{for all } n \in \mathbb{N}. \tag{4.26}$$

Combining (4.25) and (4.26), we obtain $P_{\theta^*}(\bar{y}) = p^*$, i.e. $\bar{y} \in \mathcal{A}(\theta^*, p^*)$ and thus $\partial\mathcal{B}(\theta^*, p^*) \subseteq \mathcal{A}(\theta^*, p^*)$.

Analogously, one can prove $\partial\mathcal{C}(\theta^*, p^*) \subseteq \mathcal{A}(\theta^*, p^*)$.

Let us now prove (iii). The existence of two collections of disjoint open intervals $\{(a_i, b_i)\}_{i=1}^{N_{\mathcal{B}}}$ and $\{(c_j, d_j)\}_{j=1}^{N_{\mathcal{C}}}$ such that (4.21) and (4.22) hold, with $a_i, b_i \in \partial(\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y))$ for all $i \in \{1, \dots, N_{\mathcal{B}}\}$, and $c_j, d_j \in \partial(\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y))$ for all $j \in \{1, \dots, N_{\mathcal{C}}\}$ is a direct consequence of the fact that the sets $\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)$ and $\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)$ are open (see for instance, Ref. 2). Moreover, using (ii) and the fact that $\partial(y_{\mathcal{A}} + Y) = \{y_{\mathcal{A}}, y_{\mathcal{A}} + |Y|\} \subseteq \mathcal{A}(\theta^*, p^*)$, we get $a_i, b_i, c_j, d_j \in \mathcal{A}(\theta^*, p^*)$ for all $i \in \{1, \dots, N_{\mathcal{B}}\}, j \in \{1, \dots, N_{\mathcal{C}}\}$.

It remains to show (4.23) and (4.24). Since $\mathcal{M}(\theta^*) = \gamma$, the function θ^* is Y -periodic and the optimality condition (4.8) holds, we have

$$\gamma|Y| = \int_Y \theta^* = \int_{y_{\mathcal{A}}+Y} \theta^* \geq \int_{\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}}+Y)} \theta^* = |\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)|$$

and

$$\begin{aligned} (1 - \gamma)|Y| &= \int_Y (1 - \theta^*) = \int_{y_{\mathcal{A}}+Y} (1 - \theta^*) \\ &\geq \int_{\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}}+Y)} (1 - \theta^*) = |\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)|. \quad \square \end{aligned}$$

Thanks to the decomposition given in Lemma 4.1, we can now give a new expression for J on the set Θ_γ :

Proposition 4.2. *For any $(\theta^*, p^*) \in \Theta_\gamma \times \mathbb{R}$ such that (4.8) holds and $y_{\mathcal{A}} \in \mathcal{A}(\theta^*, p^*)$, we have the expression*

$$J(\theta^*) = \frac{q^2}{12|Y|} \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \left[(1 - \gamma)^2 \sum_{i=1}^{N_{\mathcal{B}}} (b_i - a_i)^3 + \gamma^2 \sum_{j=1}^{N_{\mathcal{C}}} (d_j - c_j)^3 \right], \tag{4.27}$$

where $a_i, b_i, c_j, d_j, N_{\mathcal{B}}$ and $N_{\mathcal{C}}$ are given in Lemma 4.1. In particular, above expression is valid at maximizers θ^* .

Proof. Let us first multiply Eq. (4.5) by X_{θ^*} , then we integrate by parts. We have

$$\begin{aligned} J(\theta^*) &= \mathcal{M}((X_{\theta^*})^2) = -\frac{1}{2q(\frac{1}{\alpha_1} - \frac{1}{\alpha_0})} \mathcal{M}\left(\frac{dP_{\theta^*}}{dy} X_{\theta^*}\right) \\ &= \frac{1}{2q(\frac{1}{\alpha_1} - \frac{1}{\alpha_0})} \mathcal{M}\left(P_{\theta^*} \frac{dX_{\theta^*}}{dy}\right). \end{aligned}$$

Now, due to Eq. (3.1) and the fact that $\mathcal{M}(P_{\theta^*}) = 0$, we obtain

$$J(\theta^*) = \frac{1}{2} \mathcal{M}(P_{\theta^*} \theta^*).$$

Adding and subtracting p^* , we get

$$J(\theta^*) = \frac{1}{2} [\mathcal{M}((P_{\theta^*} - p^*)\theta^*) + p^* \gamma].$$

Since $\mathcal{M}(P_{\theta^*}) = 0$, one can rewrite p^* as follows:

$$p^* = -\mathcal{M}(P_{\theta^*} - p^*),$$

which yields

$$J(\theta^*) = \frac{1}{2} \mathcal{M}((P_{\theta^*} - p^*)(\theta^* - \gamma)).$$

Using the definitions of the sets $\mathcal{A}(\theta^*, p^*)$, $\mathcal{B}(\theta^*, p^*)$, and $\mathcal{C}(\theta^*, p^*)$, the optimality condition (4.8) and the fact that $P_{\theta^*}(\cdot)$ is Y -periodic, the previous expression of $J(\theta^*)$ becomes

$$\begin{aligned} J(\theta^*) &= \frac{1}{2|Y|} \left[(1 - \gamma) \int_{\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)} (P_{\theta^*}(y) - p^*) dy \right. \\ &\quad \left. - \gamma \int_{\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)} (P_{\theta^*}(y) - p^*) dy \right]. \end{aligned} \tag{4.28}$$

Using the decompositions (4.21) and (4.22) of the sets $\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)$ and $\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)$, we have

$$\int_{\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)} (P_{\theta^*}(y) - p^*) dy = \sum_{i=1}^{N_{\mathcal{B}}} \int_{a_i}^{b_i} (P_{\theta^*}(y) - p^*) dy$$

and

$$\int_{\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y)} (P_{\theta^*}(y) - p^*) dy = \sum_{j=1}^{N_{\mathcal{C}}} \int_{c_j}^{d_j} (P_{\theta^*}(y) - p^*) dy,$$

respectively.

In each interval (a_i, b_i) and (c_j, d_j) (with $i \in \{1, \dots, N_{\mathcal{B}}\}$, $j \in \{1, \dots, N_{\mathcal{C}}\}$) we differentiate Eq. (4.5), then using (3.1), for all $y \in (a_i, b_i) \cup (c_j, d_j)$ we get

$$-\frac{d^2 P_{\theta^*}(y)}{dy^2} = -2q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) + 2q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \left(\frac{\theta^*(y)}{\alpha_1} + \frac{1 - \theta^*(y)}{\alpha_0} \right).$$

Now, due to the optimality condition (4.8) we obtain

$$-\frac{d^2 P_{\theta^*}(y)}{dy^2} = \begin{cases} 2q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \left(\frac{1}{\alpha_1} - \frac{1}{q} \right) & \forall y \in (a_i, b_i), \\ 2q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \left(\frac{1}{\alpha_0} - \frac{1}{q} \right) & \forall y \in (c_j, d_j). \end{cases}$$

Then, since the identities (2.8) and (2.9) hold, we can write

$$-\frac{d^2 P_{\theta^*}(y)}{dy^2} = \begin{cases} 2(1 - \gamma)q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 & \forall y \in (a_i, b_i), \\ -2\gamma q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 & \forall y \in (c_j, d_j). \end{cases} \tag{4.29}$$

Since $a_i, b_i, c_j, d_j \in \mathcal{A}(\theta^*, p^*)$, we have the following boundary conditions:

$$P_{\theta^*}(y) - p^* = 0 \quad \forall y \in \{a_i, b_i, c_j, d_j\}.$$

Now, we integrate Eq. (4.29) and use the above boundary conditions to obtain

$$P_{\theta^*}(y) - p^* = \begin{cases} (1 - \gamma)q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 (y - a_i)(b_i - y) & \forall y \in (a_i, b_i), \\ -\gamma q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 (y - c_j)(d_j - y) & \forall y \in (c_j, d_j), \end{cases}$$

and hence,

$$\begin{aligned} \int_{a_i}^{b_i} (P_{\theta^*}(y) - p^*) dy &= (1 - \gamma)q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \frac{(b_i - a_i)^3}{6}, \\ \int_{c_j}^{d_j} (P_{\theta^*}(y) - p^*) dy &= -\gamma q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \frac{(d_j - c_j)^3}{6}. \end{aligned}$$

Now, summing over i , and then over J , we get

$$\int_{\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{B}} + Y)} (P_{\theta^*}(y) - p^*) dy = \frac{(1 - \gamma)}{6} q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \sum_{i=1}^{N_{\mathcal{B}}} (b_i - a_i)^3$$

and

$$\int_{\mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{C}} + Y)} (P_{\theta^*}(y) - p^*) dy = -\frac{\gamma}{6} q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \sum_{j=1}^{N_{\mathcal{C}}} (d_j - c_j)^3.$$

The result (4.27) is a direct consequence of the previous two expressions and the identity (4.28). □

4.3.3. Maximum of J

Let us now prove the identity (3.5) and the last assertion given in Theorem 3.1. To this end, we first use Proposition 4.2 in order to rewrite $J(\theta^*)$, $\theta^* \in \Theta_\gamma$ as follows:

$$\begin{aligned}
 J(\theta^*) = & \frac{q^2}{12}|Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \left[(1-\gamma)^2 \gamma^3 \sum_{i=1}^{N_B} \left(\frac{b_i - a_i}{\gamma|Y|} \right)^3 \right. \\
 & \left. + \gamma^2 (1-\gamma)^3 \sum_{j=1}^{N_C} \left(\frac{d_j - c_j}{(1-\gamma)|Y|} \right)^3 \right].
 \end{aligned}
 \tag{4.30}$$

Then, due to inequalities (4.23) and (4.24) from Lemma 4.1, we deduce the following bound for all $\theta^* \in \Theta_\gamma$:

$$J(\theta^*) \leq \frac{q^2}{12} \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \left[\gamma \sum_{i=1}^{N_B} \frac{b_i - a_i}{\gamma|Y|} + (1-\gamma) \sum_{j=1}^{N_C} \frac{d_j - c_j}{(1-\gamma)|Y|} \right],
 \tag{4.31}$$

which implies

$$J(\theta^*) \leq \frac{q^2}{12} \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \quad \forall \theta^* \in \Theta_\gamma.
 \tag{4.32}$$

Let us now prove that there exists maximizer $\theta^*_{\max} \in \Theta_\gamma$ such that

$$J(\theta^*_{\max}) = \frac{q^2}{12} \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2.
 \tag{4.33}$$

For this purpose, we consider the function θ^*_{\max} defined as follows

$$\theta^*_{\max}(y) = \begin{cases} 1 & \text{if } y \in [0, \gamma|Y|], \\ 0 & \text{if } y \in (\gamma|Y|, |Y|]. \end{cases}
 \tag{4.34}$$

Being a characteristic function, clearly $\theta^*_{\max} \in \mathcal{C}_\gamma$. Many objects introduced above (such as the state $X_{\theta^*_{\max}}$, the adjoint state $P_{\theta^*_{\max}}$, etc.) can now be computed explicitly. In fact, integrating Eqs. (3.1) and (4.5), we get

$$X_{\theta^*_{\max}}(y) = q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \cdot \begin{cases} (1-\gamma) \left(y - \frac{\gamma}{2}|Y| \right) & \text{in } [0, \gamma|Y|], \\ \gamma \left(\frac{(1+\gamma)}{2}|Y| - y \right) & \text{in } [\gamma|Y|, |Y|], \end{cases}$$

and

$$P_{\theta^*_{\max}}(y) = q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \cdot \begin{cases} \frac{\gamma(1-\gamma)(1-2\gamma)}{6} |Y|^2 \\ \quad + (1-\gamma)y(\gamma|Y| - y) & \forall y \in [0, \gamma|Y|], \\ \frac{\gamma(1-\gamma)(1-2\gamma)}{6} |Y|^2 \\ \quad - \gamma(y - \gamma|Y|)(|Y| - y) & \forall y \in [\gamma|Y|, |Y|]. \end{cases}$$

Note that the state associated with the maximizer θ^*_{\max} is piecewise linear and the adjoint state is piecewise quadratic. Taking

$$p^*_{\max} = q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \frac{\gamma(1-\gamma)(1-2\gamma)}{6} |Y|^2,$$

it is clear that the optimality condition (4.8) holds. Hence, we deduce that $\theta^*_{\max} \in \Theta_\gamma$. Let us now evaluate $J(\theta^*_{\max})$ using Proposition 4.2 with the choice $y_{\mathcal{A}} = 0$, $N_{\mathcal{B}} = N_{\mathcal{C}} = 1$, $a_1 = 0$, $b_1 = c_1 = \gamma|Y|$, and $d_1 = |Y|$. We get

$$J(\theta^*_{\max}) = \frac{q^2}{12|Y|} \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 [(1-\gamma)^2 \gamma^3 |Y|^3 + \gamma^2 (1-\gamma)^3 |Y|^3].$$

Then, we conclude that θ^*_{\max} satisfies (4.33).

Using (4.32) and (4.33) we obtain

$$\max_{\theta^* \in \Theta_\gamma} J(\theta^*) = \frac{1}{12} q^2 \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2.$$

Let us remember that all maximizers of J over \mathcal{D}_γ must be inside Θ_γ as a consequence of optimality condition (4.8) and so $\max_{\theta \in \mathcal{D}_\gamma} J(\theta) = \max_{\theta^* \in \Theta_\gamma} J(\theta^*)$. Thus, we get (3.5).

It is surprising to find a classical microstructure θ^*_{\max} as a maximizer. It follows that $J(\theta^*_{\max}) = J_0(\theta^*_{\max}) = \frac{1}{12} q^2 \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2$.

4.3.4. Uniqueness of maximizer

We have seen in Sec. 4.2 that minimizer is unique. Regarding maximizer, we can assert that all maximizers are equal to θ^*_{\max} modulo a translation given by $y_{\mathcal{A}}$. Indeed, if θ^* is any maximizer, then $\theta^* \in \Theta_\gamma$ and equality holds in (4.31). This means that we must have $N_{\mathcal{B}} = N_{\mathcal{C}} = 1$ and $b_1 - a_1 = \gamma|Y|$ and $d_1 - c_1 = (1-\gamma)|Y|$. (See passage from (4.30) to (4.31).) Then (4.21) and (4.22) become

$$\mathcal{B}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y) = (a_1, b_1) \quad \text{and} \quad \mathcal{C}(\theta^*, p^*) \cap (y_{\mathcal{A}} + Y) = (c_1, d_1).$$

Recalling the optimality condition (4.8), we obtain $\theta^* = 1$ in (a_1, b_1) and $\theta^* = 0$ in (c_1, d_1) . Thus, θ^* is a Y -periodic characteristic function of an interval of length $\gamma|Y|$. This proves our assertion.

5. Proof of Second Main Result

In this section, we prove Theorem 3.2. First of all, using the fact that the characteristic function θ^*_{\max} , defined in (4.34), belongs to the set \mathcal{C}_γ , it is clear that

$$-\frac{1}{12}q^3\gamma^2(1-\gamma)^2|Y|^2\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2 = -qJ(\theta^*_{\max}) \in \{d(\chi) : \chi \in \mathcal{C}_\gamma\}.$$

Therefore, it is enough to prove that

$$\left(-\frac{1}{12}q^3\gamma^2(1-\gamma)^2|Y|^2\left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0}\right)^2, 0\right) \subseteq \{d(\chi) : \chi \in \mathcal{C}_\gamma\}. \tag{5.1}$$

To this end, the idea is to reproduce the structure of the maximizer given by (4.34) at finer scales. Microstructure behind the maximizer was somewhat simple whereas this is not the case with other points of the interval $I = I(\alpha_0, \alpha_1, \gamma)$. The construction depends on parameters $n \in \mathbb{N}^*$ and $\delta \in (0, 1)$. First, we consider a regular partition of the interval Y formed by n intervals $I_k = [\frac{k-1}{n}|Y|, \frac{k}{n}|Y|]$, with $k \in \{1, \dots, n\}$. Each interval I_k is partitioned into two subintervals whose lengths are $\frac{1-\delta}{n}|Y|$ and $\frac{\delta}{n}|Y|$, respectively. Each of these subintervals is, in turn, partitioned into two subintervals of lengths $(\gamma\frac{1-\delta}{n}|Y|, (1-\gamma)\frac{1-\delta}{n}|Y|)$, and $(\gamma\frac{\delta}{n}|Y|, (1-\gamma)\frac{\delta}{n}|Y|)$. This process divides I_k into four subintervals: $I_k = [a_{2k-1}, b_{2k-1}] \cup [c_{2k-1}, d_{2k-1}] \cup [a_{2k}, b_{2k}] \cup [c_{2k}, d_{2k}]$ with endpoints defined by the following real numbers (see Fig. 1):

$$a_{2k-1} = \frac{k-1}{n}|Y|, \quad b_{2k-1} = c_{2k-1} = a_{2k-1} + \frac{\gamma(1-\delta)}{n}|Y|,$$

$$d_{2k-1} = a_{2k} = \frac{k-\delta}{n}|Y|, \quad b_{2k} = c_{2k} = a_{2k} + \frac{\gamma\delta}{n}|Y|, \quad d_{2k} = \frac{k}{n}|Y|.$$

Using these notations, let us define a characteristic function $\theta^*_{n,\delta}$ by

$$\theta^*_{n,\delta}(y) = \begin{cases} 1 & \text{if } y \in \bigcup_{i=1}^{2n} [a_i, b_i], \\ 0 & \text{if } y \in \bigcup_{j=1}^{2n} (c_j, d_j). \end{cases} \tag{5.2}$$

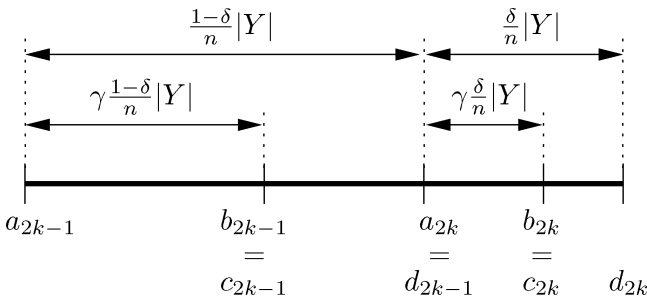


Fig. 1. Subdivision of interval $I_k = [\frac{k-1}{n}|Y|, \frac{k}{n}|Y|]$.

It is clear that $\theta_{n,\delta}^* \in \mathcal{C}_\gamma$. In order to compute the functional $J(\theta_{n,\delta}^*)$ using Proposition 4.2, first we prove that $\theta_{n,\delta}^* \in \Theta_\gamma$. For this purpose, we integrate Eqs. (3.1) and (4.5) to obtain the state, the adjoint state, etc.:

$$X_{\theta_{n,\delta}^*}(y) = q \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right) \cdot \begin{cases} (1-\gamma) \left(y - \frac{a_i + b_i}{2} \right) & \text{in } (a_i, b_i), i \in \{1, \dots, 2n\}, \\ \gamma \left(\frac{c_j + d_j}{2} - y \right) & \text{in } (c_j, d_j), j \in \{1, \dots, 2n\}, \end{cases}$$

and

$$P_{\theta_{n,\delta}^*}(y) = q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \frac{\gamma(1-\gamma)(1-2\gamma)}{6n^2} (1-3\delta+3\delta^2) |Y|^2 + q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \cdot \begin{cases} (1-\gamma)(y-a_i)(b_i-y) & \text{in } (a_i, b_i), i \in \{1, \dots, 2n\}, \\ -\gamma(y-c_j)(d_j-y) & \text{in } (c_j, d_j), j \in \{1, \dots, 2n\}. \end{cases}$$

Once again, observe the following facts: the state is piecewise linear and the adjoint state is piecewise quadratic albeit in smaller intervals. Taking

$$p_{n,\delta}^* = q^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2 \frac{\gamma(1-\gamma)(1-2\gamma)}{6n^2} (1-3\delta+3\delta^2) |Y|^2,$$

we see that the optimality condition (4.8) holds for $(\theta_{n,\delta}^*, p_{n,\delta}^*)$. Hence, $\theta_{n,\delta}^* \in \Theta_\gamma$.

Let us now use Proposition 4.2 in the particular case $N_\emptyset = N_\ell = 2n$ and we obtain

$$J(\theta_{n,\delta}^*) = \frac{1-3\delta+3\delta^2}{n^2} \max_{\theta \in \mathcal{D}_\gamma} J(\theta).$$

This formula shows that fixing $n \in \mathbb{N}^*$, and varying $\delta \in (0, 1)$, the following identity holds:

$$\{J(\theta_{n,\delta}^*) : \delta \in (0, 1)\} = \left[\frac{1}{4n^2} \max_{\theta \in \mathcal{D}_\gamma} J(\theta), \frac{1}{n^2} \max_{\theta \in \mathcal{D}_\gamma} J(\theta) \right].$$

Now, if we vary $n \in \mathbb{N}^*$, we get

$$\{J(\theta_{n,\delta}^*) : n \in \mathbb{N}^*, \delta \in (0, 1)\} = \left(0, \max_{\theta \in \mathcal{D}_\gamma} J(\theta) \right),$$

that is,

$$\begin{aligned} \{d(\theta_{n,\delta}^*) : n \in \mathbb{N}^*, \delta \in (0, 1)\} &= \left(-q \max_{\theta \in \mathcal{D}_\gamma} J(\theta), 0 \right) \\ &= \left(-\frac{1}{12} q^3 \gamma^2 (1-\gamma)^2 |Y|^2 \left(\frac{1}{\alpha_1} - \frac{1}{\alpha_0} \right)^2, 0 \right). \end{aligned}$$

Since $\{d(\theta_{n,\delta}^*) : n \in \mathbb{N}^*, \delta \in (0, 1)\} \subseteq \{d(\chi) : \chi \in \mathcal{C}_\gamma\}$, we get the inclusion (5.1) and by consequence, we conclude the proof of Theorem 3.2.

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