The zero-order Gamma-limit of the simple shear problem in nonlinear Cosserat elasticity

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Abstract

The zero-order Gamma-limit of vanishing internal length scale is studied for the mechanical energy of a shear problem in geometrically nonlinear Cosserat elasticity. The convergence of the minimizers is shown and the limit functional is characterized. One main result is that Gamma-limit and pointwise limit of the energy only coincide when $\mu_c = 0$ and are different otherwise.

Key words: Cosserat theory, Gamma-limit, micropolar, generalized continuum

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1. The Cosserat model in simple shear

We investigate the deformation of an infinite layer of material in 3D with unit height, fixed at the bottom and sheared in e_1-direction with amount $0 < \gamma < 2$ at the upper face, cf. Fig 1. Within a geometrically non-linear Cosserat theory, [11, 13, 14], the mechanical behaviour of the material can be modelled with the help of the standard deformation map $\varphi : \widehat{\Omega} \to \mathbb{R}^3$ and the tensor field of orthogonal micro-rotations $R : \widehat{\Omega} \to \mathrm{SO}(3)$, describing the translation and independent rotation of a material point, respectively. Here, $\widehat{\Omega} \subset \mathbb{R}^3$ is the reference configuration. By $\mu > 0$ we denote the standard elastic shear modulus, $\mu_c \geq 0$ is the Cosserat couple modulus, $\lambda \in \mathbb{R}$ the second elastic Lamé parameter, $a_1 \geq 0$, $a_2 \geq 0$, $a_3 \geq 0$ are non-dimensional constants; $L_c > 0$ is the characteristic length scale.

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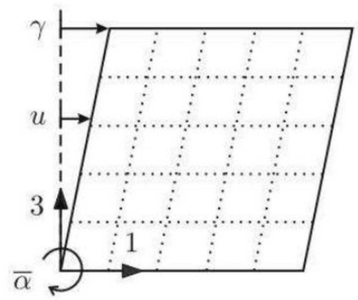

Figure 1: The deformed state exhibits a homogeneous region in the interior of the structure which motivates the kinematics of simple shear.

A detailed discussion about the physical meaning of these parameters and its relation to other models can be found in the review article [26].

The deformed material is characterized by the minimizers (φ, R) of the isotropic mechanical energy

$$\begin{aligned} E_{3D}(\varphi, R) &= \int_{\widehat{\Omega}} \mu\left|\operatorname{sym}(\overline{U} - \mathbb{1}_3)\right|^2 + \mu_c\left|\operatorname{skew}(\overline{U} - \mathbb{1}_3)\right|^2 + \frac{\lambda}{4}\Big[(\det \overline{U} - 1)^2 + \Big(\frac{1}{\det \overline{U}} - 1\Big)^2\Big] \\ &\quad + \mu\frac{L_c^2}{2}\Big(a_1\left|\operatorname{dev}\operatorname{sym} R^T \operatorname{Curl} R\,\right|^2 + a_2\left|\operatorname{skew} R^T \operatorname{Curl} R\right|^2 + \frac{a_3}{3}\operatorname{tr}(R^T \operatorname{Curl} R)^2\Big)\,\mathrm{d}x \\ &= \int_{\widehat{\Omega}} W_{\mathrm{mp}}(\overline{U}) + W_{\mathrm{disloc}}(R^T \operatorname{Curl} R)\,\mathrm{d}x\,, \qquad \overline{U} = R^T \mathrm{D}\varphi \end{aligned} \tag{1}$$

subject to certain boundary conditions, see [3, 27, 26, 30, 31, 6, 5, 8] for further information and [17] for a comparison to experiments.

The symmetry of the boundary conditions and the infinite extension in e_1-direction lead to the reduced kinematics

$$\varphi(x_1, x_2, x_3) = \begin{pmatrix} x_1 + u(x_3) \\ x_2 \\ x_3 \end{pmatrix}\,, \qquad F = \mathrm{D}\varphi(x_1, x_2, x_3) = \begin{pmatrix} 1 & 0 & u'(x_3) \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}\,, \tag{2}$$

with $u(0) = 0$ and $u(1) = \gamma$. The microrotations $R \in \mathrm{SO}(3)$ satisfy the identity

$$R(x_1, x_2, x_3) = \begin{pmatrix} \cos\alpha(x_3) & 0 & \sin\alpha(x_3) \\ 0 & 1 & 0 \\ -\sin\alpha(x_3) & 0 & \cos\alpha(x_3) \end{pmatrix} \tag{3}$$

with fixed axis of rotation e_2, implying

$$\mathrm{Curl} R = \begin{pmatrix} 0 & -\sin\alpha(x_3)\alpha'(x_3) & 0 \\ 0 & 0 & 0 \\ 0 & -\cos\alpha(x_3)\alpha'(x_3) & 0 \end{pmatrix}. \tag{4}$$

From now on, we denote x_3 by x and set

$$\Omega := (0,1) \subset \mathbb{R}.$$

The deformation u introduced in (2) and the local rotation angle α around the axis $x_3 = x$ in (3) permit to re-write the functional E_{3D} in a simpler form, see [3]. The solutions to the 3D-shear problem can thus be obtained as minimizers of the *mechanical energy functional* and the *reduced mechanical energy functional*

$$\begin{aligned} E(u,\alpha) &= \frac{\mu}{2}\int_0^1 4L_c^2|\alpha'|^2 + |u'|^2 + \Big(\sin(\alpha)u' - 4\sin^2\big(\frac{\alpha}{2}\big)\Big)^2 \,\mathrm{d}x \\ &\quad + \frac{\mu_c}{2}\int_0^1 \Big(\cos(\alpha)u' - 2\sin(\alpha)\Big)^2 \,\mathrm{d}x, \qquad (5) \\ \widehat{E}(u,\alpha) &= \frac{\mu}{2}\int_0^1 4L_c^2|\alpha'|^2 + |u'|^2 + [\alpha(\alpha - u')]^2 \,\mathrm{d}x + \frac{\mu_c}{2}\int_0^1 \Big(\frac{2-\alpha^2}{2}u' - \frac{6\alpha - \alpha^3}{3}\Big)^2 \,\mathrm{d}x. \qquad (6) \end{aligned}$$

The functional $\widehat{E}(u,\alpha)$ is obtained from $E(u,\alpha)$ in (5) after introducing the third-order expansions $\cos(\alpha) \sim 1 - \frac{\alpha^2}{2}$, $\sin(\alpha) \sim \alpha - \frac{\alpha^3}{6}$ and dropping all higher order terms except $\frac{\mu_c}{2}\Big(\frac{\alpha^4}{4}|u'|^2 - \frac{1}{3}\alpha^5 u' + \frac{1}{9}\alpha^6\Big)$ to finally get a complete quadratic form.

In this article we are concerned with the zero-order Gamma-limit of vanishing internal length scale L_c of $E(u,\alpha)$. However, the methods of this article are also applicable to the Gamma-limit $L_c \searrow 0$ of $\widehat{E}(u,\alpha)$ and we expect that Gamma-limit to be very similar to the one obtained in this paper as long as α is small.

Formally writing $L_c = \frac{\varepsilon}{\sqrt{2\mu}}$ for $\varepsilon \geq 0$ leads to

$$E_\varepsilon(u,\alpha) := \begin{cases} \int_0^1 \varepsilon^2|\alpha'|^2 + \frac{\mu}{2}|u'|^2 + W(u',\alpha)\,\mathrm{d}x, & \text{if } (u,\alpha) \in (W^{1,2}(\Omega))^2, \\ +\infty, & \text{else} \end{cases} \tag{7}$$

with the potential

$$W(u',\alpha) := \frac{\mu}{2}\Big(\underbrace{\sin(\alpha)u' - 4\sin^2\big(\frac{\alpha}{2}\big)}_{=\sin(\alpha)u' + 2\cos(\alpha) - 2}\Big)^2 + \frac{\mu_c}{2}\Big(\cos(\alpha)u' - 2\sin(\alpha)\Big)^2. \tag{8}$$

By $W^{m,2}(\Omega)$ we denote the Sobolev space of m-times weakly differentiable functions in $L^2(\Omega)$. Let $C^\infty_\#(\Omega;\mathbb{R})$ denote the smooth functions $g:\Omega\to\mathbb{R}$ with $g(0)=g(1)$ and let $W^{1,2}_\#(\Omega;\,\mathbb{R})$ be the closure of $C^\infty_\#(\Omega;\,\mathbb{R})$ with respect to the $W^{1,2}$-norm, i.e. the Sobolev functions $g\in W^{1,2}(\Omega)$ with identical traces at the boundary. The minimization of E in (5) is carried out in the reflexive Banach space

$$\mathcal{X} := \mathcal{X}_u\times\mathcal{X}_\alpha := \Big\{u\in W^{1,2}(\Omega;\,\mathbb{R})\,\Big|\,u(0)=0,\ u(1)=\gamma\Big\}\times\Big\{\alpha\in W^{1,2}_\#(\Omega;\,[0,2\pi])\Big\}. \tag{9}$$

The function $W(u',\cdot)$ is 2π-periodic in α. Motivated by numerical considerations, see [7], (9) confines the range of α to $[0,2\pi]$. The interval $[0,2\pi]$ is only one possible choice but determines the analysis for the entire article. Below, in Figures 2, 4 and 5, other ranges of α will be displayed if it is advantageous for the presentation.

The concept of Gamma-convergence describes the asymptotic behaviour of a family of minimization problems. It is arguably the most natural way to study the convergence of variational problems as it supplies information not only of the minimizers itself, but also of the convergence of the variational problems. Theorem 1 below states the circumstances.

The characterization of the zero-order Gamma-limit of E_ε allows to qualitatively and quantitatively understand the model for small characteristic length scale L_c which would otherwise demand simulations with ultra-high spatial resolution. Clearly, the Gamma-limit differs from the pointwise limit. This is illustrated in the following non-commutative diagram. It is a well-known result from Gamma-convergence, cf. e.g. [16][Prop.5.7], that a non-increasing family of functionals Gamma-converges toward the lower semicontinuous envelope of its pointwise limit $\widetilde{E_0}$, i.e. $E_0=\mathrm{lsc}(\widetilde{E_0})$. The task in this article is hence similar to that of [12] and [23], see also [4] for a discrete setting.

$$\begin{array}{ccc} E_\varepsilon & \xrightarrow{\varepsilon\to 0} & \widetilde{E}_0 \\ {\scriptstyle \Gamma\text{–}\lim_{\varepsilon\to 0}}\big\downarrow & \not\!\!/\!\!/_{\neq} & \\ E_0 & & \end{array}$$

The Gamma-limit functional E_0 of E_ε will be identified in Proposition 1. For comparison, the limit functional $\widetilde{E}_0$ for $L_c\searrow 0$ differs in general from E_0 and is simply (cf. Eqn. (5))

$$\widetilde{E}_0(u,\alpha) := \frac{\mu}{2}\int_0^1 |u'|^2+\Big(\sin(\alpha)u'-4\sin^2\big(\frac{\alpha}{2}\big)\Big)^2\,\mathrm{d}x+\frac{\mu_c}{2}\int_0^1\Big(\cos(\alpha)u'-2\sin(\alpha)\Big)^2\,\mathrm{d}x. \tag{10}$$

The condensed energy $E^{\mathrm{cond}}(u):=\min_\alpha \widetilde{E}_0(u,\alpha)$ can be determined explicitly, see the appendix. Accordingly, the limit $L_c\searrow 0$ of the full functional in 3D is

$$\widetilde{E}_{3D}(\varphi,R)=\int_{\widehat{\Omega}}\mu\big|\mathrm{sym}(\overline{U}-\mathbb{1}_3)\big|^2+\mu_c\big|\mathrm{skew}(\overline{U}-\mathbb{1}_3)\big|^2+\frac{\lambda}{4}\Big[(\det\overline{U}-1)^2+\Big(\frac{1}{\det\overline{U}}-1\Big)^2\Big]\,\mathrm{d}x \tag{11}$$

and the condensed energy $E_{3D}^{\rm cond}(\varphi) := \min_{R\in{\rm SO}(3)} \widetilde{E}_{3D}(\varphi, R)$ can also be determined explicitly. At this point, we are unable to compute the Gamma-limit $L_c \searrow 0$ of the full three-dimensional functional $\widetilde{E}_{3D}$ which is why we restrict ourselves here to the analysis of the shear problem.

The paper is organized in the following way. In Section 2 we recall the theory of Gamma-convergence as needed later. Section 3 deals with the zero-order Gamma-limit of E as $L_c \searrow 0$. Here also the minimizers of E are classified depending on the values of μ, μ_c and the amount of shear γ. In the appendix we compare the zero-order Gamma-limit with the pointwise minimization of E for $L_c = 0$.

As a good starting point and for gaining first insights into the concepts of this article, we consider for fixed u' the term $\widehat{W}(\alpha) := \frac{\mu}{2}\big[\alpha(\alpha - u')\big]^2$ from Eqn. (6), see Fig. 2. It is a double-well potential with minima at $\alpha = 0$ and $\alpha = u'$ and a maximum at $\alpha = \frac{u'}{2}$. Similar potentials have been used for a long time to model phase transitions and segmentation phenomena, see, e.g., [18]. (Recent articles on phase separation commonly replace the quartic polynomial by a logarithmic expression closer to the correct physical free energy).

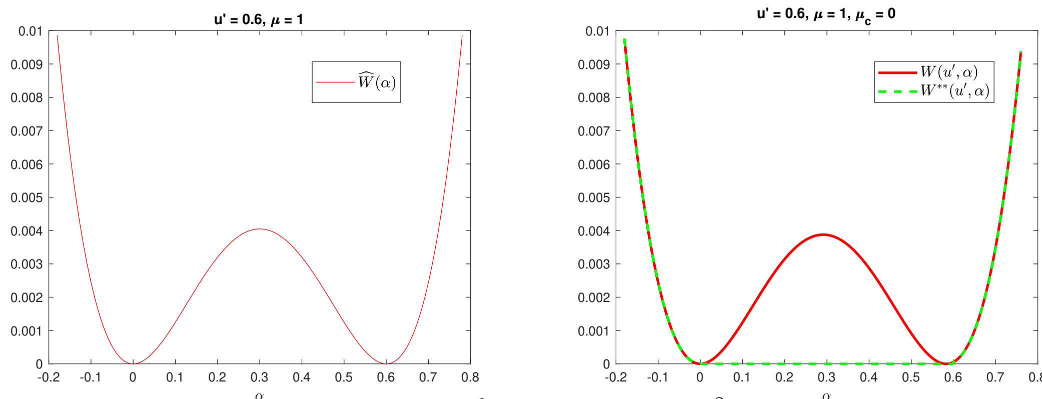

Figure 2: Comparison of the reduced energy $\widehat{W}(\alpha) = \frac{\mu}{2}\big[\alpha(\alpha - u')\big]^2$ (left) and the full energy W (right) together with its convexification W^{**} for $\mu = 1$, $\mu_c = 0$, $u' = 0.6$ and $\alpha \in [-0.2, 0.8]$.

In the region separating the two minima, $\widehat{W}$ is positive, thereby forming an energy barrier, also called surface energy. This is the minimal amount of energy that must be provided to let the physical system pass between the optimal states $\alpha = 0$ and $\alpha = u'$. A related concept is the activation energy of chemical reactions in an Arrhenius type equation, see, e.g., [24].

The energy barrier models analytically the resilience of the material to changes of the inner molecular structure needed to pass from the state $\alpha = 0$ to the state $\alpha = u'$. The associated molecular or atomistic restructuring can mathematically be formulated as Markov processes, see, e.g., [22].

Since $\widehat{W}$ originates from W by a third-order Taylor expansion, one may expect that also W displays a double well. Indeed, within a certain range of μ and μ_c, this is the case. Fig. 2 compares W and $\widehat{W}$ for one set of parameters with striking similarity.

If a double-well structure of W and $\widehat{W}$ is present, minimizing sequences develop fine scale oscillations. For further explanations, we refer to [25] and references therein.

The zero-order Gamma-limit goes along with a convexification of W. This convexification connects the minima and removes the energy barrier. Using this convexified energy E_0, cf. Eqn. (16), should lead to a significant improvement in the numerical simulations.

Fig. 2 shows only a part of W. Interestingly, the double well is very flat and located in a tiny section of the full graph of W that may easily be overlooked, cf. Fig. 5.

2. Theory of Gamma-convergence

We restrict the presentation of Gamma-convergence to metric spaces (X, d) as we do not wish to differentiate between properties that hold only sequentially or more generally. Convergences stated below are always with regard to d and the Gamma-limit will depend on that metric. If Gamma-convergence is defined on a general topological space X this space must fulfil the first axiom of countability.

Definition 1. *Let (X, d) be a metric space. A family of functionals $(G_n)_{n\in\mathbb{N}} : X \to \overline{\mathbb{R}} := \mathbb{R} \cup \{-\infty, +\infty\}$* Gamma-converges *for $n \to \infty$ to $G : X \to \overline{\mathbb{R}}$, if the following two conditions are met:*

(i) (liminf inequality)
For all $x \in X$ and every sequence $(x_n)_{n\in\mathbb{N}} \subset X$ with $x_n \to x$ in X, it holds

$$G(x) \leq \liminf_{n\to\infty} G_n(x_n). \tag{12}$$

(ii) (recovery sequence)
For every $x \in X$, there exists a sequence $(x_n)_{n\in\mathbb{N}} \subset X$ with $x_n \to x$ in X such that

$$G(x) \geq \limsup_{n\to\infty} G_n(x_n).$$

Definition 2. *Let (X, d) be a metric space.*

(i) A functional $G : X \to \overline{\mathbb{R}}$ is coercive *on X if for all $\alpha \in \mathbb{R}$ the closure of the sublevel sets $\{x \in X \mid G(x) \leq \alpha\}$ is compact in X.*

(ii) A family of functionals $\{G_n\}_{n\in\mathbb{N}} : X \to \overline{\mathbb{R}}$ is equi-coercive *if there exists a lower semi-continuous coercive functional $\psi : X \to \overline{\mathbb{R}}$ such that $G_n \geq \psi$ for all $n \in \mathbb{N}$.*

If G is coercive there exists a compact set $K \subset X$ with $\inf_{x\in X} G(x) = \inf_{x\in K} G(x)$.

The choice of topology in X is crucial: The finer the topology in X, the easier the lower semicontinuity property inherent in (12) is satisfied. Contrary, the compactness of the sublevel sets K_α calls for coarser topologies. Hence, both conditions are competing. Often, the weak topology in a Sobolev space provides a good compromise where both properties are satisfied simultaneously.

Theorem 1 (Fundamental theorem of Gamma-convergence).
Let (X,d) be a metric space and $(G_n)_{n\in\mathbb{N}} : X \to \overline{\mathbb{R}}$ be an equi-coercive family of functionals. Then

(i) $\Gamma-\liminf_{n\to\infty} G_n$ *and* $\Gamma-\limsup_{n\to\infty} G_n$ *are coercive and*

$$\min_{x\in X}\big(\Gamma-\liminf_{n\to\infty} G_n(x)\big) = \liminf_{n\to\infty}\inf_{x\in X} G_n(x).$$

(ii) If in addition (G_n) Gamma-converges to G in X, then G is coercive and

$$\min_{x\in X} G(x) = \lim_{n\to\infty}\inf_{x\in X} G_n(x).$$

Proof. See, e.g., [16, Theorem 7.8]. □

Theorem 1 remains true in topological spaces X. It states in particular that while G_n need not have minima, the Gamma-limit G always attends its minimum.

3. Zero-order Gamma-limit

We derive the first term in the Gamma-expansion of E_ε. We introduce the closed domain

$$\overline{D} := [0,2]\times[0,2\pi] \subset \mathbb{R}^2. \tag{13}$$

Writing $z := u'$, let (cf. Eqn. (7))

$$Q(z,\alpha) := \begin{cases} \frac{\mu}{2}|z|^2 + W(z,\alpha), & \text{if } (z,\alpha)\in\overline{D}, \\ +\infty, & \text{else} \end{cases} \tag{14}$$

so that

$$Q(z,\alpha) = \frac{\mu}{2}|z|^2 + \frac{\mu}{2}\Big(\sin(\alpha)z - 4\sin^2\big(\frac{\alpha}{2}\big)\Big)^2 + \frac{\mu_c}{2}\Big(\cos(\alpha)z - 2\sin(\alpha)\Big)^2 \quad \text{if } (z,\alpha)\in\overline{D}.$$

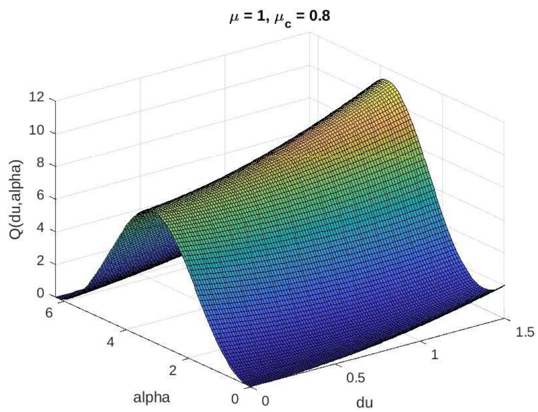

Figure 3: Plot of $Q(z,\alpha)$ for $\alpha \in [0, 2\pi]$, $z \in [0, 1.5]$, $\mu = 1$ and $\mu_c = 0.8$.

Definition 3. *For Q given by (14) we denote by Q^{**} the convex and lower-semicontinuous envelope of Q, i.e.*

$$Q^{**}(z,\alpha) := \sup\big\{g(z,\alpha) \mid g \textit{ is convex, lower semi-continuous and } g(z,\alpha) \le Q(z,\alpha)\big\}. \tag{15}$$

The computation of Q^{**} is postponed to Lemma 2 below.

We define the relaxed functional

$$E_0(u,\alpha) := \begin{cases} \int_0^1 Q^{**}(u',\alpha)\,\mathrm{d}x, & \text{if } (u,\alpha) \in \widetilde{\mathcal{X}}, \\ +\infty, & \text{else} \end{cases} \tag{16}$$

and for $\varepsilon > 0$ the family of functionals

$$E_\varepsilon(u,\alpha) := \begin{cases} \int_0^1 \varepsilon^2|\alpha'|^2 + Q(u',\alpha)\,\mathrm{d}x, & \text{if } (u,\alpha) \in \mathcal{X}, \\ +\infty, & \text{else.} \end{cases} \tag{17}$$

In (16) we introduced the Banach space

$$\widetilde{\mathcal{X}} \;:=\; \mathcal{X}_u \times C^0_\#(\overline{\Omega};\,[0,2\pi]) \tag{18}$$

The reason for introducing $\widetilde{\mathcal{X}}$ is that for $\varepsilon \searrow 0$, the term $\int_0^1 \varepsilon|\alpha'|^2\,\mathrm{d}x$ in $E_\varepsilon(u,\alpha)$ disappears, so the weak limit α of a minimizing sequence $(\alpha_n)_{n\in\mathbb{N}} \subset W^{1,2}_\#(\Omega;\,[0,2\pi])$ need not be weakly differentiable and may leave $\mathcal{X}_\alpha$.

Lemma 1. *Let $(\varepsilon_n)_{n\in\mathbb{N}}$ be a sequence of positive real numbers with $\varepsilon_n \searrow 0$ for $n \to \infty$. Then the family of functionals $(E_{\varepsilon_n})_{n\in\mathbb{N}}$ defined in (17) is equi-coercive with respect to weak convergence in $(L^2(\Omega))^2$.*

Proof. We are going to show that for every sequence $(u_n,\alpha_n)_{n\in\mathbb{N}}\subset(L^2(\Omega))^2$ with $\sup_{n\in\mathbb{N}}E_{\varepsilon_n}(u_n,\alpha_n)<\infty$ there exists a subsequence $(u_{n_k},\alpha_{n_k})_{k\in\mathbb{N}}$ that converges weakly in $(L^2(\Omega))^2$. This implies the equicoercivity of $(E_{\varepsilon_n})_{n\in\mathbb{N}}$.

Directly from (17) and (14) we obtain

$$\frac{\mu}{2}\|u_n'\|^2_{L^2(\Omega)}\leq E_{\varepsilon_n}(u_n,\alpha_n)\leq C \tag{19}$$

uniformly in $n\in\mathbb{N}$. From the definition (17) of E_{ε_n}, this implies $(u_n,\alpha_n)\in\mathcal{X}=\mathcal{X}_u\times\mathcal{X}_\alpha$ for every $n\in\mathbb{N}$. Functions $u_n\in\mathcal{X}_u$ are absolutely continuous in Ω. Employing $u_n(0)=0$, this yields $u_n(x)\leq\int_0^x u_n'(\xi)\,\mathrm{d}\xi$, so $|u_n(x)|\leq\int_0^1|u_n'(\xi)|\,\mathrm{d}\xi$ for a.e. $x\in\Omega$. Consequently,

$$\|u_n\|_{L^2(\Omega)}\ \leq\ \|u_n\|_{L^\infty(\Omega)}\ \leq\ \|u_n'\|_{L^2(\Omega)}. \tag{20}$$

This shows that $\|u_n\|_{W^{1,2}(\Omega)}$ is bounded uniformly in n. By the Banach-Alaoglu theorem, there exists a subsequence $(u_{n_k})_{k\in\mathbb{N}}$ that converges weakly in $L^2(\Omega)$.

From $(\alpha_n)_{n\in\mathbb{N}}\subset\mathcal{X}_\alpha$ follows $\alpha_n\in[0,2\pi]$ pointwise in Ω and hence the boundedness $\|\alpha_n\|_{L^2(\Omega)}\leq 2\pi$ uniformly in $n\in\mathbb{N}$. Again, (see, e.g., Theorem 2.6 in [10]) this implies the existence of a subsequence (α_{n_k}) converging to α weakly in $L^2(\Omega)$. □

Proposition 1 (Zero-order Gamma-limit). *Let $(\varepsilon_n)_{n\in\mathbb{N}}$ be a sequence of positive real numbers converging to* 0. *Let E_{ε_n} on $(L^2(\Omega))^2$ be given by (17), and as in (16)*

$$E_0(u,\alpha)=\begin{cases}\int_0^1 Q^{**}(u',\alpha)\,\mathrm{d}x, & \textit{if } (u,\alpha)\in\widetilde{\mathcal{X}},\\ +\infty, & \textit{else.}\end{cases}$$

Then E_0 is the Gamma-limit of E_{ε_n} with respect to weak convergence in $L^2(\Omega)$ for $n\to\infty$.

Proof. (i) *liminf inequality.* Let $(u,\alpha)\in(L^2(\Omega))^2$ and $(u_n,\alpha_n)_{n\in\mathbb{N}}\subset(L^2(\Omega))^2$ be a sequence with $u_n\rightharpoonup u$, $\alpha_n\rightharpoonup\alpha$ in $L^2(\Omega)$ for $n\to\infty$ and $\liminf_{n\in\mathbb{N}}E_{\varepsilon_n}(u_n,\alpha_n)<\infty$. Up to subsequences, we may assume that

$$\lim_{n\to\infty}E_{\varepsilon_n}(u_n,\alpha_n)\text{ exists and is finite} \tag{21}$$

and $(u_n,\alpha_n)\in\mathcal{X}$ for all $n\in\mathbb{N}$. From $E_{\varepsilon_n}(u_n,\alpha_n)<\infty$, as in (19) in Lemma 1, up to subsequences, we have $u_n'\rightharpoonup u'$ in $L^2(\Omega)$. The (compact) embedding $W^{1,2}(\Omega)\to C^0(\overline{\Omega})$ implies $u_n(x)\to u(x)$ pointwise for all $x\in\overline{\Omega}$. Similarly, $\alpha_n\in\mathcal{X}_\alpha$ implies $\alpha_n(x)\to\alpha(x)$ for all $x\in\overline{\Omega}$ and $\alpha\in C^0_\#(\overline{\Omega};[0,2\pi])$. From these pointwise convergences, (21) and (14) we infer $(u(x),\alpha(x))\in\overline{D}$ for all $x\in\Omega$ and $Q(u',\alpha)<\infty$. Also, $u(0)=0$, $u(1)=\gamma$, hence $(u,\alpha) \in \widetilde{\mathcal{X}}$. From $(u_n', \alpha_n) \rightharpoonup (u', \alpha)$ in $(L^2(\Omega))^2$ we find

$$\begin{aligned}
\liminf_{n\to\infty} E_{\varepsilon_n}(u_n,\alpha_n) &= \liminf_{n\to\infty} \int_0^1 \varepsilon_n^2 |\alpha_n'|^2 + Q(u_n',\alpha_n)\,\mathrm{d}x \\
&\geq \liminf_{n\to\infty} \int_0^1 \varepsilon_n^2 |\alpha_n'|^2 + Q^{**}(u_n',\alpha_n)\,\mathrm{d}x \qquad (22)\\
&\geq \int_0^1 Q^{**}(u',\alpha)\,\mathrm{d}x \;=\; E_0(u,\alpha). \qquad (23)
\end{aligned}$$

Here, (22) follows from (15) and (23) holds because Q^{**} is convex and lower semi-continuous, consequently $(u_n',\alpha_n) \mapsto \int_0^1 Q^{**}(u_n',\alpha_n)\,\mathrm{d}x$ is weakly lower semi-continuous.
(ii) *limsup inequality.* Let $(u,\alpha) \in (L^2(\Omega))^2$ be fixed. We may assume $E_0(u,\alpha) < \infty$ (otherwise the Limsup inequality is evident) such that $(u,\alpha) \in \widetilde{\mathcal{X}}$. We must prove the existence of a sequence $(u_n,\alpha_n) \subset (L^2(\Omega))^2$ with $u_n \rightharpoonup u$, $\alpha_n \rightharpoonup \alpha$ in $L^2(\Omega)$ for $n \to \infty$ and

$$E_0(u,\alpha) = \int_0^1 Q^{**}(u',\alpha)\,\mathrm{d}x \geq \limsup_{n\to\infty} E_{\varepsilon_n}(u_n,\alpha_n).$$

Because of $\limsup_{n\to\infty} E_{\varepsilon_n}(u_n,\alpha_n) \leq \int_0^1 Q(u',\alpha)\,\mathrm{d}x$ it is sufficient to show that

$$\limsup_{n\to\infty} \int_0^1 Q(u_n',\alpha_n)\,\mathrm{d}x \leq \int_0^1 Q^{**}(u',\alpha)\,\mathrm{d}x \qquad (24)$$

for a suitable recovery sequence $(u_n,\alpha_n)_{n\in\mathbb{N}}$. Subsequently we approximate u by piecewise affine functions u_n with $u_n(0)=0$, $u_n(1)=\gamma$ for all $n \in \mathbb{N}$ and α by piecewise constant functions periodic in Ω. The set of such (u_n,α_n) approximates $\widetilde{\mathcal{X}}$ densely in $(L^2(\Omega))^2$.

<u>Case 1</u>: Let $[a,b] \subset \Omega$ be an interval where $u' = z \equiv \text{const}$, $\alpha \equiv \text{const}$ in $[a,b]$. Fix $\varepsilon > 0$. Then there exist $x_\varepsilon \in (0,1)$ and $(z_\varepsilon^1,\alpha_\varepsilon^1) \in \mathbb{R}^2$, $(z_\varepsilon^2,\alpha_\varepsilon^2) \in \mathbb{R}^2$ with

$$\begin{aligned}
x_\varepsilon Q(z_\varepsilon^1,\alpha_\varepsilon^1) + (1-x_\varepsilon) Q(z_\varepsilon^2,\alpha_\varepsilon^2) &\leq Q^{**}(z,\alpha) + \varepsilon, \\
\|x_\varepsilon (z_\varepsilon^1,\alpha_\varepsilon^1) + (1-x_\varepsilon)(z_\varepsilon^2,\alpha_\varepsilon^2) - (z,\alpha)\| &< \varepsilon.
\end{aligned} \qquad (25)$$

The existence of such x_ε, $(z_\varepsilon^1,\alpha_\varepsilon^1)$, $(z_\varepsilon^2,\alpha_\varepsilon^2)$ follows from

$$\begin{aligned}
Q^{**}(z,\alpha) = \inf \Big\{ & \liminf_{m\to\infty} x_m Q(z_m^1,\alpha_m^1) + (1-x_m) Q(z_m^2,\alpha_m^2) \mid x_m \in (0,1), \\
& \lim_{m\to\infty} x_m (z_m^1,\alpha_m^1) + (1-x_m)(z_m^2,\alpha_m^2) = (z,\alpha) \Big\}.
\end{aligned}$$

Construct an affine function u_ε with constant derivative $u'_\varepsilon(x) \equiv z_\varepsilon := x_\varepsilon z_\varepsilon^1 + (1 - x_\varepsilon) z_\varepsilon^2$, where $u_\varepsilon(0) = 0$ if $a = 0$ and $u_\varepsilon(1) = \gamma$ if $b = 1$, as well as the constant function $\alpha_\varepsilon(x) :\equiv x_\varepsilon \alpha_\varepsilon^1 + (1 - x_\varepsilon)\alpha_\varepsilon^2$ for $x \in \Omega$. Let

$$v_\varepsilon(x) := \begin{cases} z_\varepsilon^1, & \text{for } 0 \le x \le x_\varepsilon, \\ z_\varepsilon^2, & \text{for } x_\varepsilon < x \le 1 \end{cases} \qquad w_\varepsilon(x) := \begin{cases} \alpha_\varepsilon^1, & \text{for } 0 \le x \le x_\varepsilon, \\ \alpha_\varepsilon^2, & \text{for } x_\varepsilon < x \le 1 \end{cases} \tag{26}$$

extended 1-periodically to functions for $x \in \mathbb{R}$ and define the $1/n$-periodic functions

$$z_n^\varepsilon(x) := v_\varepsilon(nx), \qquad \alpha_n^\varepsilon(x) := w_\varepsilon(nx).$$

It holds $z_n^\varepsilon = (u_n^\varepsilon)' \rightharpoonup z_\varepsilon = u'_\varepsilon$ and $\alpha_n^\varepsilon \rightharpoonup \alpha_\varepsilon$ in $L^2(\Omega)$ for $n \to \infty$, cf. [10, Example 2.5], where the piecewise affine functions u_n^ε are constructed as u_ε was above, e.g. $(u_n^\varepsilon)' = z_n^\varepsilon$ and $u_n^\varepsilon(0) = 0$ if $a = 0$, $u_n^\varepsilon(1) = \gamma$ if $b = 1$. Formally, the limsup-inequality also requires $u_n^\varepsilon \rightharpoonup u_\varepsilon$ in $L^2(\Omega)$. Indeed, from $(u_n^\varepsilon)' \rightharpoonup u'_\varepsilon$, integration by parts yields

$$\int_0^1 (u_n^\varepsilon(x) - u_\varepsilon(x))\phi'(x)\,\mathrm{d}x \to 0 \qquad \text{for } n \to \infty \tag{27}$$

and any $\phi \in C_0^\infty(\Omega)$. Formally replacing ϕ' in (27) by a new test function ζ, from the density of the continuous functions in $L^2(\Omega)$, this yields $u_n^\varepsilon \rightharpoonup u_\varepsilon$ in $L^2(\Omega)$ for $n \to \infty$.

Finally, by construction,

$$\lim_{n\to\infty} \int_a^b Q(z_n^\varepsilon, \alpha_n^\varepsilon)\,\mathrm{d}x = (b-a)\big[x_\varepsilon Q(z_\varepsilon^1, \alpha_\varepsilon^1) + (1-x_\varepsilon) Q(z_\varepsilon^2, \alpha_\varepsilon^2)\big] \le \int_a^b Q^{**}(z,\alpha)\,\mathrm{d}x + \varepsilon(b-a).$$

Taking the limit $\varepsilon \searrow 0$ this yields the desired limsup-inequality.

Case 2: u is piecewise affine, α is piecewise constant.

We may assume that u' and α are discontinuous at identical points in Ω. Now repeat the construction of Case 1 on each interval where u' and α are continuous. □

For the computation of Q^{**}, we need to consider the minimizers and the minimal energy $\underline{e}_{\mu,\mu_c}$ of E_0 (defined in (7)),

$$\underline{e}_{\mu,\mu_c} := \min\left\{ E_0(u,\alpha) \,\middle|\, (u,\alpha) \in \widetilde{\mathcal{X}} \right\}.$$

Table 1 below has the details.

Parameters	Minimizers	Minimal energy $\underline{e}_{\mu,\mu_c}$ of E_0
$\mu_c = 0$	$(\overline{u}, \alpha_1^- = 0)$, $(\overline{u}, \alpha_1^+ = 2\arctan(\frac{\gamma}{2}))$	$\frac{\mu}{2}\gamma^2$
$\mu = \mu_c$	$(\overline{u}, \alpha_2)$	$\mu(\gamma^2 + 4 - 2\sqrt{\gamma^2+4})$
$\mu \neq \mu_c$, if $\alpha_1^\pm$ exists	$(\overline{u}, \alpha_1^-)$, $(\overline{u}, \alpha_1^+)$	$\frac{\mu+\mu_c}{2}\gamma^2 - \frac{2\mu_c^2}{\lvert\mu-\mu_c\rvert}$
$\mu \neq \mu_c$, else	$(\overline{u}, \alpha_2)$	$\mu\big(\gamma^2 + 4 - 2\sqrt{\gamma^2+4}\big)$

Table 1: Unique minimizers of E_0 in $\widetilde{\mathcal{X}}$ and minimal energies for different parameter ranges. The case $\mu_c = 0$ is a special case of the third regime $\mu \neq \mu_c$ and existing $\alpha_1^\pm$, see Remark 1. The case $\mu = \mu_c$ is a special case of the fourth regime $\mu \neq \mu_c$ and non-existing $\alpha_1^\pm$. Explanations regarding the existence of $\alpha_1^\pm$ and a characterization of the third and fourth regime are found in Remark 2.

We adopt the notations

$$\overline{u}(x) := \gamma\, x, \qquad 0 \leq x \leq 1 \tag{28}$$

for the *homogeneous deformation* which turns out to be optimal in $\mathcal{X}_u$, and set

$$\alpha_1^- := \arctan\Big(\frac{\mu\gamma - f}{2\mu + \frac{\gamma}{2}f}\Big), \quad \alpha_1^+ := \arctan\Big(\frac{\mu\gamma + f}{2\mu - \frac{\gamma}{2}f}\Big), \quad \alpha_2 := \arctan\Big(\frac{\gamma}{2}\Big) \tag{29}$$

for the global minimizers of E_0, where

$$f := \Big((\gamma^2+4)(\mu-\mu_c)^2 - 4\mu^2\Big)^{1/2}. \tag{30}$$

Remark 1. *The case $\mu_c = 0$ is a limiting case of the third regime $\mu \neq \mu_c$ and existing $\alpha_1^\pm$. For $\mu_c = 0$, by Eqn. (30), $f = \gamma\mu$ such that by Formula (29)*

$$\alpha_1^- = 0, \qquad \alpha_1^+ = \arctan\Big(\frac{4\gamma}{4-\gamma^2}\Big). \tag{31}$$

This formula had already been derived in [3]. Therein, the value α_1^+ for $\mu_c = 0$ had been denoted α_3 and introduced by the identity

$$\alpha_3 = \eta^{-1}(\gamma), \qquad \eta(\alpha) := \frac{4\sin^2\big(\frac{\alpha}{2}\big)}{\sin(\alpha)}. \tag{32}$$

The inverse $\eta^{-1}(\gamma)$ in (32) exists for $\gamma \in [0, \pi)$ while α_1^+ in (31) is evaluated for $\gamma \in [0, 2]$. Due to

$$\eta(\alpha) = \frac{4\sin^2\big(\frac{\alpha}{2}\big)}{\sin(\alpha)} = \frac{2\sin^2\big(\frac{\alpha}{2}\big)}{\sin\big(\frac{\alpha}{2}\big)\cos\big(\frac{\alpha}{2}\big)} = 2\tan\Big(\frac{\alpha}{2}\Big),$$

Eqn. (32) can be rewritten to (only valid when $\mu_c = 0$*)*

$$\alpha_1^+ = \eta^{-1}(\gamma) = 2\arctan\Big(\frac{\gamma}{2}\Big) = 2\,\alpha_2, \tag{33}$$

improving (31). The identity $\arctan\left(\frac{4\gamma}{4-\gamma^2}\right) = 2\arctan\Big(\frac{\gamma}{2}\Big)$ *can also be obtained directly from the addition theorem*

$$\arctan(v_1) + \arctan(v_2) = \arctan\Big(\frac{v_1 v_2}{1 - v_1 v_2}\Big) \qquad \textit{for } v_1 v_2 \leq 1$$

after setting $v_1 = v_2 := \frac{\gamma}{2}$*.*

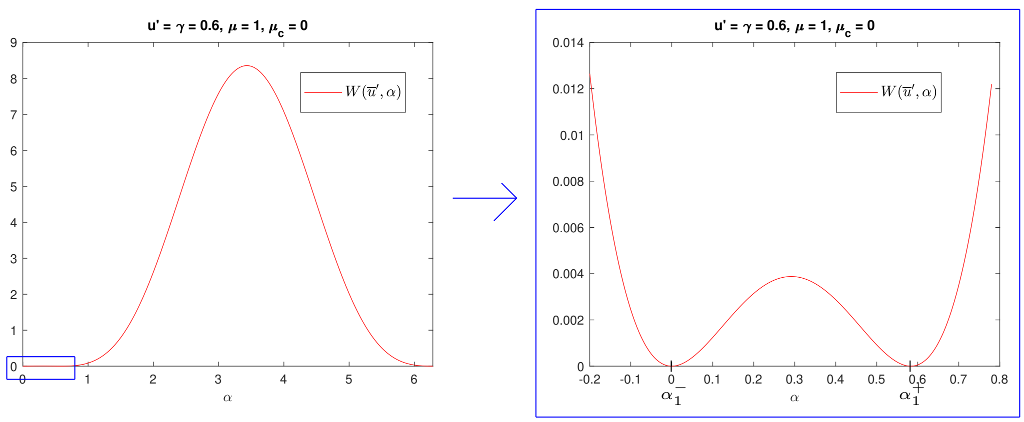

Figure 4: Two plots of $\alpha \mapsto W(\gamma, \alpha)$ for $\mu_c = 0$, $\mu = 1$ and $\gamma = 0.6$. Left: Plot for $\alpha \in [0, 2\pi]$. Right: Close-up for $\alpha \in [-0.2, 0.8]$ showing a double well with minima at $\alpha_1^- = 0$ and $\alpha_1^+ = 2\arctan(\frac{\gamma}{2}) \approx 0.5829$ as predicted by Eqn. (33). The double well is very flat and does not show up in the full plot on the left.

For $\mu_c < \mu$, $\alpha_1^\pm$ exists if $\mu_c \leq \mu_c^{\mathrm{crit}}$ with μ_c^{crit} defined by Eqn. (37), see Remark 2 below. For $\mu \leq \mu_c$, $\alpha_1^\pm$ exists if $\mu \neq \mu_c$ and $\mu_c \geq \mu_c^{\mathrm{crit}}$, where μ_c^{crit} is now defined by (39).

Fig. 5 displays one example for the case $\mu > \mu_c$. In the interval $\alpha \in [0, 1]$ which contains all minimizers, $W(\gamma, \cdot)$ is strictly convex for $\mu_c > \mu_c^{\mathrm{crit}}$, while for $\mu_c = 0$ and in the non-classical regime $\mu_c \leq \mu_c^{\mathrm{crit}}$, $W(\gamma, \cdot)$ is a double-well potential with minimizers at α_1^- and at α_1^+, cf. Fig. 5.

The limiting case $\mu_c = 0$ is displayed in Fig. 4.

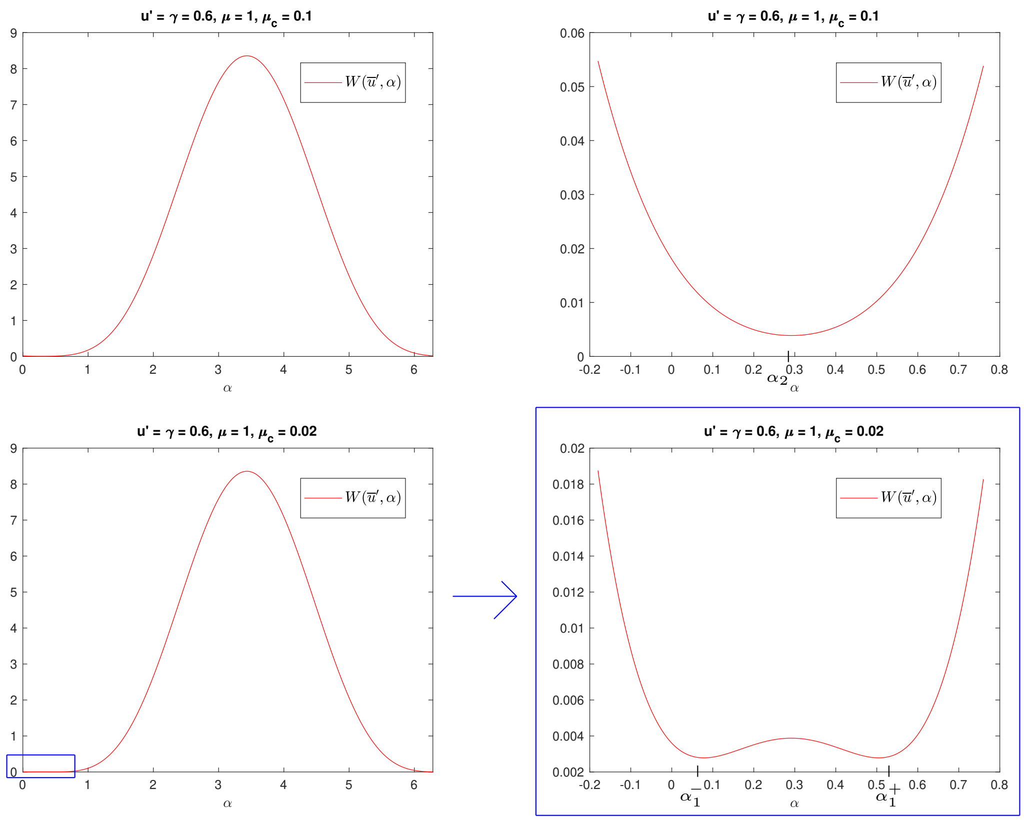

Figure 5: Plots of $\alpha \mapsto W(\gamma, \alpha)$ for $\mu = 1$ and $\gamma = 0.6$. Left: Plots for $\alpha \in [0, 2\pi]$. Right: Close-ups for $\alpha \in [-0.2, 0.8]$. Bottom: For $\mu_c = 0.02 < \mu_c^{\text{crit}} = 0.0422$ there is a double well with minimal value $\underline{e}_{\mu,\mu_c} = \frac{\mu_c}{2}\gamma^2 - \frac{2\mu_c^2}{\mu - \mu_c} \approx 0.00278$ at $\alpha_1^- \approx 0.0783$ and at $\alpha_1^+ \approx 0.5046$ in accordance with Eqn. (29). Top: Strict convexity in the interval $\alpha \in [0, 1]$ for $\mu_c = 0.1 > \mu_c^{\text{crit}}$ with the unique minimal value $\underline{e}_{\mu,\mu_c} = \mu\big[\frac{\gamma^2}{2} + 4 - 2\sqrt{\gamma^2 + 4}\big] \approx 0.003877$ at $\alpha_2 = \arctan(\gamma/2) \approx 0.2915$. The double well is very flat and practically invisible in the full plot displayed on the bottom line left. The blue box on the bottom left illustrates the section which is enlarged on the right.

The data of Table 1 is computed for fixed γ. For the variational problem at hand, we write $z := \overline{u}' = \gamma$ and have from now on $\alpha_1^\pm = \alpha_1^\pm(z)$, $\alpha_2 = \alpha_2(z)$ and $f = f(z)$.

Remark 2 (Existence of $\alpha_1^\pm(z)$ and different regimes). *Whenever $\alpha_1^\pm$ exist, these are the unique global minimizers of E_0. In [3], $\alpha_1^\pm$ have been computed as solutions of*

$$z\sin(\alpha) + 2\cos(\alpha) = \frac{2\mu}{\mu - \mu_c}. \tag{34}$$

Writing $S := \sin(\alpha)$, $C := \cos(\alpha)$, $g := \frac{2\mu}{\mu-\mu_c}$, we find $2C = g - zS$ and $4C^2 = 4(1-S^2) = (g-zS)^2$, leading to the quadratic equation

$$S^2 - \frac{2zg}{z^2+4}S + \frac{g^2-4}{z^2+4} = 0.$$

The solutions $S^\pm$ and hence $\alpha_1^\pm$ exist provided $\mu \neq \mu_c$ and $d := (z^2+4-g^2)^{1/2} = \frac{f(z)}{|\mu-\mu_c|}$ is real-valued, where $f = f(z) := \big((z^2+4)(\mu-\mu_c)^2 - 4\mu^2\big)^{1/2}$, cf. Eqn. (30). We introduce for $\mu \neq \mu_c$ and $2\mu \geq \mu_c$ the critical value of z *by*

$$z_{\mathrm{crit}} := \frac{2}{|\mu-\mu_c|}\sqrt{\mu_c(2\mu-\mu_c)}, \qquad \textit{in particular} \qquad z_{\mathrm{crit}}^2 + 4 = \frac{4\mu^2}{(\mu-\mu_c)^2}. \tag{35}$$

It holds $f(z_{\mathrm{crit}}) = 0$. Hence the case $z = z_{\mathrm{crit}}$ constitutes a transition point with

$$\alpha_1^-(z_{\mathrm{crit}}) = \alpha_1^+(z_{\mathrm{crit}}) = \alpha_2(z_{\mathrm{crit}}) = \arctan\Big(\frac{z_{\mathrm{crit}}}{2}\Big). \tag{36}$$

<u>1. Case</u>: $\mu_c < \mu$.
We adopt temporarily the symbol μ_c^{crit} from [3] for the critical value of μ_c *and define*

$$\mu_c^{\mathrm{crit}} = \mu_c^{\mathrm{crit}}(z) := \mu\Big(1 - \frac{2}{\sqrt{z^2+4}}\Big). \tag{37}$$

For $\mu_c < \mu$, the existence of $\alpha_1^\pm$ and the third regime of Table 1 are characterized by the condition $\mu_c \leq \mu_c^{\mathrm{crit}}$ ensuring that d is real-valued. This can be rewritten using (35) to a condition $z \geq z_{\mathrm{crit}}$, i.e.

$$\begin{aligned}\mu_c \leq \mu_c^{\mathrm{crit}}(z) &\iff \mu_c \leq \mu\Big(1-\frac{2}{\sqrt{z^2+4}}\Big) \iff \frac{2}{\sqrt{z^2+4}} \leq \frac{\mu-\mu_c}{\mu} \iff \frac{4\mu^2}{(\mu-\mu_c)^2} \leq z^2+4 \\ &\iff \frac{4(\mu^2-(\mu-\mu_c)^2)}{(\mu-\mu_c)^2} \leq z^2 \iff \frac{2}{\mu-\mu_c}\sqrt{\mu^2-(\mu-\mu_c)^2} \leq z \\ &\iff \frac{2}{\mu-\mu_c}\sqrt{\mu_c(2\mu-\mu_c)} \leq z \iff z_{\mathrm{crit}} \leq z. \end{aligned} \tag{38}$$

2. Case: $\mu \le \mu_c$. For $\mu = \mu_c$, Eqn. (34) has no solution. Let $\mu < \mu_c$. The critical value of μ_c is then

$$\mu_c^{\text{crit}} = \mu_c^{\text{crit}}(z) := \mu\Big(1 + \frac{2}{\sqrt{z^2+4}}\Big). \tag{39}$$

For $\mu < \mu_c$, as in the first case, $\alpha_1^{\pm}$ solves (34) provided $\mu_c^{\text{crit}} \le \mu_c$. We assume that

$$\mu \ge \frac{\mu_c}{2}. \tag{40}$$

Then the third regime of Table 1 for $\mu < \mu_c$ is characterized by

$$\begin{aligned}
\mu_c^{\text{crit}}(z) \le \mu_c &\iff \mu\Big(1 + \frac{2}{\sqrt{z^2+4}}\Big) \le \mu_c \iff \frac{2}{\sqrt{z^2+4}} \le \frac{\mu_c - \mu}{\mu} \iff \frac{4\mu^2}{(\mu_c-\mu)^2} \le z^2 + 4 \\
&\iff \frac{4(\mu^2 - (\mu_c-\mu)^2)}{(\mu_c-\mu)^2} \le z^2 \iff \frac{2}{\mu_c-\mu}\sqrt{\mu^2 - (\mu_c-\mu)^2} \le z \\
&\iff \frac{2}{\mu_c-\mu}\sqrt{\mu_c(2\mu-\mu_c)} \le z \iff z_{\text{crit}} \le z.
\end{aligned} \tag{41}$$

In both cases, we find that $\alpha_1^{\pm}$ exist if $z_{\text{crit}} \le z$. For $\mu = \mu_c$, z_{crit} is undefined and the minimizers $\alpha_1^{\pm}$ do not exist.

Under the assumption (40) we may repeat Table 1, now written in terms of z.

Parameters	Minimizers	Minimal energy $\underline{e}_{\mu,\mu_c}(z)$ of E_0
$\mu_c = 0$	$(\overline{u}, \alpha_1^- = 0)$, $(\overline{u}, \alpha_1^+(z) = 2\arctan(\frac{z}{2}))$	$\frac{\mu}{2}z^2$
$\mu = \mu_c$	$(\overline{u}, \alpha_2(z))$	$\mu(z^2 + 4 - 2\sqrt{z^2+4})$
$\mu \ne \mu_c$, $z_{\text{crit}} \le z$	$(\overline{u}, \alpha_1^-(z))$, $(\overline{u}, \alpha_1^+(z))$	$\frac{\mu+\mu_c}{2}z^2 - \frac{2\mu_c^2}{\lvert\mu-\mu_c\rvert}$
$\mu \ne \mu_c$, $z_{\text{crit}} > z$	$(\overline{u}, \alpha_2(z))$	$\mu\big(z^2 + 4 - 2\sqrt{z^2+4}\big)$

Table 2: The data of Table 1 for different values of z.

To complete the discussion of the zero-order Gamma-limit, it remains to compute the convexification Q^{**}. Motivated by Eqn. (31) valid only for $z \le 2$, we restrict in the following to $z \in [0, 2]$.

Lemma 2 (Computation of Q^{**}). *Let Q be given by (14), $0 \le z \le 2$, $\mu_c \le 2\mu$ and let*

$$\underline{e}_{\mu,\mu_c}(z) := \begin{cases} \mu\big(z^2+4-2\sqrt{z^2+4}\big) & \text{if } (\mu=\mu_c) \text{ or } (z_{\text{crit}} > z), \\ \frac{\mu+\mu_c}{2}z^2 - \frac{2\mu_c^2}{|\mu-\mu_c|} & \text{else.} \end{cases} \tag{42}$$

For $f(z) := \big((z^2+4)(\mu-\mu_c)^2 - 4\mu^2\big)^{1/2}$, let

$$\alpha_1^-(z) := \arctan\Big(\frac{\mu z - f(z)}{2\mu + \frac{z}{2}f(z)}\Big), \alpha_1^+(z) := \arctan\Big(\frac{\mu z + f(z)}{2\mu - \frac{z}{2}f(z)}\Big), \alpha_2(z) := \arctan\Big(\frac{z}{2}\Big). \tag{43}$$

Then, depending on μ and μ_c, for $0 \le z \le 2$, $0 \le \alpha \le 2\pi$, the convexification $Q^{**}(z,\alpha)$ is given by the following formulas.

(i) If $\mu_c = 0$:

$$Q^{**}(z,\alpha) = \frac{\mu}{2}z^2. \tag{44}$$

(ii) If $\mu = \mu_c$:

$$Q^{**}(z,\alpha) = \begin{cases} W(z,\alpha) + \frac{\mu}{2}z^2 & \text{if } \alpha \in [0,\alpha_2(z)], \\ \big(\mu z^2 - \underline{e}_{\mu,\mu_c}(z)\big)\frac{\alpha-\alpha_2(z)}{2\pi-\alpha_2(z)} + \underline{e}_{\mu,\mu_c}(z) & \text{if } \alpha \in [\alpha_2(z), 2\pi] \end{cases}. \tag{45}$$

(iii) If $\mu_c \ne \mu$:

$$Q^{**}(z,\alpha) = \begin{cases} W(z,\alpha) + \frac{\mu}{2}z^2 & \text{if } (\alpha \in [0,\alpha_1^-(z)) \text{ and } z \ge z_{\text{crit}}) \\ & \quad \text{or } (\alpha \in [0,\alpha_2(z)) \text{ and } z < z_{\text{crit}}), \\ \underline{e}_{\mu,\mu_c}(z) & \text{if } \alpha \in [\alpha_1^-(z), \alpha_1^+(z)) \text{ and } z \ge z_{\text{crit}}, \\ \big(\frac{\mu+\mu_c}{2}z^2 - \underline{e}_{\mu,\mu_c}(z)\big)\frac{\alpha-\alpha_1^+(z)}{2\pi-\alpha_1^+(z)} + \underline{e}_{\mu,\mu_c}(z) & \text{if } \alpha \in [\alpha_1^+(z), 2\pi] \text{ and } z \ge z_{\text{crit}}, \\ \big(\frac{\mu+\mu_c}{2}z^2 - \underline{e}_{\mu,\mu_c}(z)\big)\frac{\alpha-\alpha_2(z)}{2\pi-\alpha_2(z)} + \underline{e}_{\mu,\mu_c}(z) & \text{if } \alpha \in [\alpha_2(z), 2\pi] \text{ and } z < z_{\text{crit}}. \end{cases} \tag{46}$$

Remark 3. *Eqn. (46) is the general formula for Q^{**} and contains both (44) and (45) as limiting or special cases. To see this, for $\mu_c = 0$, it holds $z_{\text{crit}} = 0$ by (35), $\underline{e}_{\mu,\mu_c}(z) = \frac{\mu}{2}z^2$ by (42), $f(z) = \mu z$ which implies $\alpha_1^-(z) = 0$ by Eqn. (43). Hence, for $(z,\alpha) \in \overline{D}$, Eqn. (46) simplifies to (44).*

For $\mu = \mu_c$, $\alpha_1^{\pm}$ are undefined. Formally replacing z_{crit} in Eqn. (46) by $+\infty$ as the limiting value of z_{crit} in Eqn. (35) for $\mu \to \mu_c$ then leads to Formula (45).

Proof. To compute the convex envelope of the continuous function Q in the closed domain $\overline{D} := [0,2]\times[0,2\pi]$, the following two formulas are helpful. For $(z,\alpha) \in \overline{D}$, we have

$$Q^{**}(z,\alpha) = \min_{t\in[0,1]} \Big\{ tQ(z_1,\alpha_1) + (1-t)Q(z_2,\alpha_2) \;\Big|\; tz_1 + (1-t)z_2 = z,\; t\alpha_1 + (1-t)\alpha_2 = \alpha \Big\},$$
$$Q^{**}(z,\alpha) = \sup \big\{ l(z,\alpha) \;\big|\; l \le Q \text{ in } \overline{D}, l \text{ is affine} \big\}.$$

Furthermore,

$$\frac{\partial^2 Q}{\partial z^2}(z,\alpha) = \mu\big[1 + \sin^2(\alpha)\big] + \mu_c \cos^2(\alpha) > 0,$$

implying that $z \mapsto Q(z,\alpha)$ is strictly convex.

Part (1): Explicit construction of an underestimator $l(z,\alpha)$.

In general, the determination of the convex envelope is a difficult task. Let $l(z,\alpha)$ denote the function defined by the right of (46), and set for $(z,\alpha) \in \overline{D}$

$$L(z,\alpha) := l(z,\alpha) - \frac{\mu}{2} z^2. \tag{47}$$

Due to (14), for $(z,\alpha) \in \overline{D}$, it holds

$$Q(z,\alpha) = \frac{\mu}{2} z^2 + W(z,\alpha).$$

Hence L is an underestimator of W while l is an underestimator of Q. Subsequently, the function $L(z,\alpha)$ is constructed by connecting the local minimizers of $W(z,\cdot)$ for fixed z by a function affine in α. Once L is constructed, l is obtained from (47).

The minimizers of $W(z,\cdot)$ for fixed z can be read off from Table 2 and Eqn. (29) or (43). Consider first the special case (i) with $\mu_c = 0$. Here, for fixed z, the three points $(\alpha_1^-, W(z,\alpha_1^-)) = (0,0)$, $(\alpha_1^+(z), W(z,\alpha_1^+(z))) = \big(2\arctan\big(\frac{z}{2}\big), 0\big)$ and $(2\pi, W(z,2\pi)) = (2\pi, 0)$ where $W(z,\cdot)$ has minimal energy $\underline{e}_{\mu,\mu_c} - \frac{\mu}{2}z^2 = 0$ are connected. This leads to the lower bound $L \equiv 0$ of W corresponding to $l(z,\alpha) = \frac{\mu}{2}z^2$ and eventually with Part (2)–Part (5) below to $Q^{**}(z,\alpha) = \frac{\mu}{2}z^2$, e.g. Eqn. (44). See Fig. 8 for a visualization of this case and Fig. 3 for a plot of $Q(z,\alpha)$.

Now consider (ii) with $\mu = \mu_c$. For $\alpha \in [0, \alpha_2(z)]$, $W(z,\cdot)$ is convex, resulting in $L(z,\alpha) = W(z,\alpha)$ and Eqn. $(45)_1$. For $\alpha \in [\alpha_2(z), 2\pi]$, the points $(\alpha_2(z), W(z,\alpha_2))$ and $(2\pi, W(z,2\pi))$ are connected by a function affine in α which results in Eqn. $(45)_2$.

In the case (iii) with $\mu \neq \mu_c$, when $z < z_{\text{crit}}$, the construction is as in (ii). When $z \geq z_{\text{crit}}$, $W(z, \cdot)$ is convex in $[0, \alpha_1^-(z))$, leading to $(46)_1$. For $\alpha \in [\alpha_1^-(z), \alpha_1^+(z)]$, $W(z, \cdot)$ forms a double-well potential. Connecting by a function affine in α the two minima

$$\begin{aligned}
(\alpha_1^-(z), W(z, \alpha_1^-(z))) &= \Big(\alpha_1^-(z), \underline{e}_{\mu,\mu_c}(z) - \frac{\mu}{2} z^2\Big), \\
(\alpha_1^+(z), W(z, \alpha_1^+(z))) &= \Big(\alpha_1^+(z), \underline{e}_{\mu,\mu_c}(z) - \frac{\mu}{2} z^2\Big)
\end{aligned} \tag{48}$$

leads to Eqn. $(46)_2$. For $\alpha \in [\alpha_1^+(z), 2\pi]$, the convexification of $W(z, \cdot)$ is an affine function connecting $(\alpha_1^+(z), W(z, \alpha_1^+(z))) = (\alpha_1^+(z), \underline{e}_{\mu,\mu_c}(z) - \frac{\mu}{2} z^2)$ and the end point $(2\pi, W(z, 2\pi)) = (2\pi, W(z, 0)) = (2\pi, \frac{\mu_c}{2} z^2)$, yielding $(46)_3$. This ends the construction of $L(z, \alpha)$ and completely defines $l(z, \alpha) = L(z, \alpha) + \frac{\mu}{2}|z|^2$.

It remains to validate that this function $l(z, \alpha)$ is indeed the convex and lower semicontinuous envelope of Q for $(z, \alpha) \in \overline{D}$, i.e. that it is convex, less or equal Q and greater or equal any convex underestimator of Q. We focus on the most general case (iii) with $\mu \neq \mu_c$ and $l(z, \alpha)$ given by the right of (46).

Part (2): Convexity of $l_i(z, \alpha)$ on A_i.
Even though $l(z, \alpha)$ is separately convex in z and in α, we still need to prove the joint convexity of l as a function of two variables. Let (cf. the right hand side of Eqn. (46))

$$\begin{aligned}
&l_1(z,\alpha) := \begin{cases} W(z,\alpha) + \frac{\mu}{2} z^2, & \text{if } (z,\alpha) \in A_1, \\ +\infty, & \text{else}, \end{cases} \qquad l_2(z,\alpha) := \begin{cases} \underline{e}_{\mu,\mu_c}(z), & \text{if } (z,\alpha) \in A_2, \\ +\infty, & \text{else}, \end{cases} \\
&l_3(z,\alpha) := \begin{cases} \big(\frac{\mu+\mu_c}{2} z^2 - \underline{e}_{\mu,\mu_c}(z)\big) \frac{\alpha - \alpha_1^+(z)}{2\pi - \alpha_1^+(z)} + \underline{e}_{\mu,\mu_c}(z) & \text{if } (z,\alpha) \in A_3, \\ +\infty, & \text{else}, \end{cases} \\
&l_4(z,\alpha) := \begin{cases} \big(\frac{\mu+\mu_c}{2} z^2 - \underline{e}_{\mu,\mu_c}(z)\big) \frac{\alpha - \alpha_2(z)}{2\pi - \alpha_2(z)} + \underline{e}_{\mu,\mu_c}(z) & \text{if } (z,\alpha) \in A_4, \\ +\infty, & \text{else} \end{cases}
\end{aligned} \tag{49}$$

for the sets (cf. $(46)_1$ to $(46)_4$)

$$\begin{aligned}
A_1 &:= \big\{(z,\alpha) \in \overline{D} \;\big|\; z \geq z_{\text{crit}},\ \alpha \in [0, \alpha_1^-(z))\big\} \cup \big\{(z,\alpha) \in \overline{D} \;\big|\; z < z_{\text{crit}},\ \alpha \in [0, \alpha_2(z))\big\}, \\
A_2 &:= \big\{(z,\alpha) \in \overline{D} \;\big|\; z \geq z_{\text{crit}},\ \alpha \in [\alpha_1^-(z), \alpha_1^+(z))\big\}, \\
A_3 &:= \big\{(z,\alpha) \in \overline{D} \;\big|\; z \geq z_{\text{crit}},\ \alpha \in [\alpha_1^+(z), 2\pi]\big\}, \\
A_4 &:= \big\{(z,\alpha) \in \overline{D} \;\big|\; z < z_{\text{crit}},\ \alpha \in [\alpha_2(z), 2\pi]\big\}.
\end{aligned}$$

Fig. 6 below plots the sets A_i exemplary for one set of parameters with $\mu_c < \mu$.

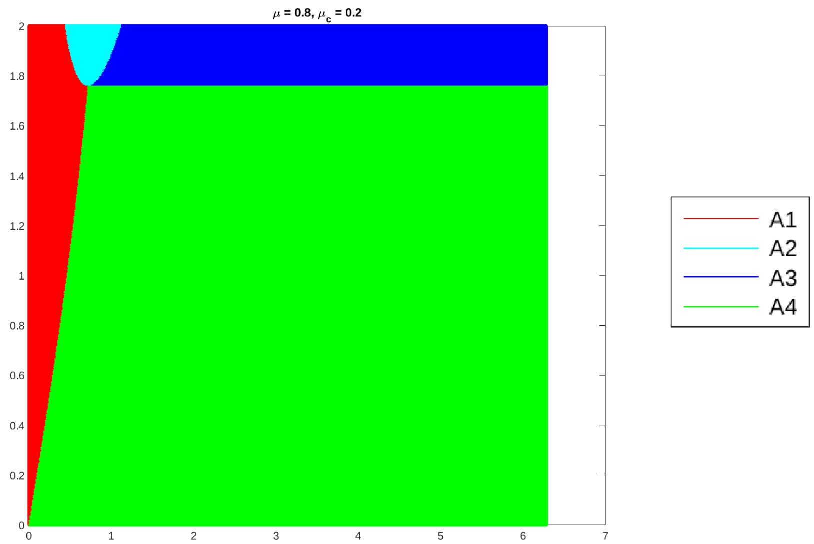

Figure 6: Plot of the sets A_i, $1 \le i \le 4$ for $\mu = 0.8$, $\mu_c = 0.2$. $\Gamma_{14} := \overline{A_1} \cap \overline{A_4}$ is not a straight line.

The convexity of $l_2(z) = \underline{e}_{\mu,\mu_c}(z)$, cf. $(46)_2$, follows at once from $l_2''(z) = \mu + \mu_c > 0$. The convexity of $l_1(z,\alpha)$ in the range A_1 follows from checking that all three principal minors of the Hessian of $W(z,\alpha) + \frac{\mu}{2}z^2$ are non-negative on A_1. These are

$$\begin{aligned}
\frac{\partial^2 l_1}{\partial^2 z}(z,\alpha) &= \mu(\sin^2(\alpha)+1) + \mu_c\cos^2(\alpha) > 0, \\
\frac{\partial^2 l_1}{\partial \alpha^2}(z,\alpha) &= 2\mu I_1(z,\alpha) + (\mu-\mu_c)\big[I_2(z,\alpha)^2 - I_1(z,\alpha)^2\big] \;=:\; I_3(z,\alpha), \qquad (50)\\
\det(D^2 l_1)(z,\alpha) &= \underbrace{\big(\mu(\sin^2(\alpha)+1)+\mu_c\cos^2(\alpha)\big)}_{>0}\underbrace{\big[2\mu I_1(z,\alpha)+(\mu-\mu_c)\big(I_2(z,\alpha)^2-I_1(z,\alpha)^2\big]}_{=I_3(z,\alpha)}.
\end{aligned}$$

Here we introduced

$$I_1(z,\alpha) \;:=\; 2\cos(\alpha) + \sin(\alpha)z, \qquad I_2(z,\alpha) \;:=\; \cos(\alpha)z - 2\sin(\alpha). \tag{51}$$

It can be checked that on A_1

$$I_1(z,\alpha) \ge 0, \qquad I_2(z,\alpha)^2 - I_1(z,\alpha)^2 \ge I_1(z,\alpha). \tag{52}$$

To prove convexity of l_1, due to (50), it remains to show $I_3(z,\alpha) \ge 0$. For $\mu_c < \mu$, this follows at once from (50). For $\mu < \mu_c$, due to (52), $(\mu-\mu_c)(I_2^2 - I_1^2) \ge (\mu-\mu_c)I_1(z,\alpha)$ such that

$$I_3(z,\alpha) \ge I_1(z,\alpha)\big[2\mu + (\mu-\mu_c)\big] \ge I_1(z,\alpha)\big[\mu_c + \mu - \mu_c\big] \ge 0,$$

where we used the assumption (40).

With (50) this demonstrates the convexity of l_1 on A_1.

To prove the convexity of l_3 on A_3, let $w(z) := \frac{2\mu z+2f(z)}{4\mu - zf(z)}$. An elementary computation shows $w'(z) \geq 0$ and $w''(z) \geq 0$ on A_3. This yields the convexity of $-\alpha_1^+(z) = -\arctan(w(z))$ as in general any composition $g_1 \circ g_2$ of two functions g_1 and g_2 is convex, provided g_1, g_2 are convex and g_2 is monotone. The convexity of $-\alpha_1^+(z)$ implies that

$$\frac{\partial^2 l_3}{\partial z^2}(z,\alpha) = \frac{2\mu_c^2}{|\mu-\mu_c|}\,\frac{2\pi-\alpha}{(2\pi-\alpha_1^+(z))^2}\left(\frac{2(\alpha_1^+(z)')^2}{2\pi-\alpha_1^+(z)} - \alpha_1^+(z)''\right) \geq 0 \quad \text{on } A_3. \tag{53}$$

Since $\frac{\partial^2 l_3}{\partial \alpha^2}(z,\alpha) = 0$ and

$$\frac{\partial^2 l_3}{\partial z \partial \alpha}(z,\alpha) = \frac{2\mu_c^2}{|\mu-\mu_c|}\big(2\pi-\alpha_1^+(z)\big)^{-2}\,\frac{w'(z)}{1+w(z)^2} \geq 0,$$

this proves the convexity of l_3 in A_3.

Finally, $\frac{\partial^2 l_4}{\partial \alpha^2}(z,\alpha) = 0$ and

$$\frac{\partial^2 l_4}{\partial z \partial \alpha}(z,\alpha) = \frac{1}{(2\pi-\alpha_2(z))^2}\,\Big[(2\pi-\alpha_2(z))\Big((\mu_c-\mu)z + \frac{2\mu z}{(z^2+4)^{1/2}}\Big) + \frac{(\mu+\mu_c)z^2 - 2\mu(z^2+4) + 4\mu(z^2+4)^{1/2}}{z^2+4}\Big]. \tag{54}$$

First let $\mu < \mu_c$. Then the first term in brackets $[\ldots]$ in (54) is clearly non-negative. For the numerator of the second term in brackets we find

$$(\mu+\mu_c)z^2 - 2\mu(z^2+4) + 4\mu(z^2+4)^{1/2} = (\mu_c-\mu)z^2 - 8\mu + 4\mu(z^2+4)^{1/2} \geq 0,$$

proving $\frac{\partial^2 l_4}{\partial z \partial \alpha}(z,\alpha) \geq 0$ on A_4 for $\mu < \mu_c$. Now let $\mu_c < \mu$. Reformulating (54), we find

$$\frac{\partial^2 l_4}{\partial z \partial \alpha}(z,\alpha) = \frac{1}{(2\pi-\alpha_2(z))^2}\,\frac{1}{z^2+4}\Big[(2\pi-\alpha_2(z))z\,I_4(z) + I_5(z)\Big] \tag{55}$$

with

$$\begin{aligned} I_4(z) &:= 2\mu(z^2+4)^{1/2} - (\mu-\mu_c)(z^2+4), \\ I_5(z) &:= (\mu+\mu_c)z^2 + 4\mu(z^2+4)^{1/2} - 2\mu(z^2+4). \end{aligned} \tag{56}$$

We estimate $I_4(z)$, $I_5(z)$ on A_4 where $0 \leq z < z_{\text{crit}}$. For $\mu_c < \mu$, we have

$$\begin{aligned} I_4(z) &= (z^2+4)^{1/2}\Big[\underbrace{2\mu - (\mu-\mu_c)(z^2+4)^{1/2}}_{> 2\mu-(\mu-\mu_c)(z_{\text{crit}}^2+4)^{1/2} \overset{(35)}{=} 2\mu-(\mu-\mu_c)\frac{2\mu}{\mu-\mu_c} = 0}\Big] > 0, \\ I_5(z) &= (\mu+\mu_c)z^2 + 2\mu(z^2+4)^{1/2}\Big[\underbrace{2-(z^2+4)^{1/2}}_{> 2-(z_{\text{crit}}^2+4)^{1/2} \overset{(35)}{=} 2-\frac{2\mu}{\mu-\mu_c} = \frac{2\mu_c}{\mu-\mu_c} \geq 0}\Big] > 0. \end{aligned}$$

Due to (55), this demonstrates $\frac{\partial^2 l_4}{\partial z \partial \alpha}(z,\alpha) > 0$ on A_4.

Lengthy computations yield

$$\frac{\partial^2 l_4}{\partial z^2}(z,\alpha) \;=\; I_6(z) + \frac{2\pi-\alpha}{(2\pi-\alpha_2(z))^2\,(z^2+4)^2}\Big[2(\mu-\mu_c)z^3 + \frac{1}{2\pi-\alpha_2(z)}I_7(z)\Big], \qquad (57)$$

where we introduced

$$\begin{aligned} I_6(z) \;&:=\frac{\alpha-\alpha_2(z)}{2\pi-\alpha_2(z)}\Big(\frac{8\mu-(\mu-\mu_c)(z^2+4)^{3/2}}{(z^2+4)^{3/2}} + \frac{2\mu[(z^2+4)^{3/2}-4]}{(z^2+4)^{3/2}}\Big)\\ &= \frac{\alpha-\alpha_2(z)}{2\pi-\alpha_2(z)}\,\frac{1}{(z^2+4)^{3/2}}\Big(8\mu+(2\mu-(\mu-\mu_c))(z^2+4)^{3/2}-8\mu\Big)\\ &= (\mu+\mu_c)\,\frac{\alpha-\alpha_2(z)}{2\pi-\alpha_2(z)} \;\geq\; 0 \qquad \text{on } A_4, \qquad (58)\\ I_7(z) \;&:= 8\mu(z^2+4)^2-4(\mu+\mu_c)z^2-16\mu(z^2+4)^{1/2}. \end{aligned}$$

First let $\mu_c < \mu$. Then, it holds on A_4

$$\begin{aligned} I_7(z) \;&=\; 8\mu(z^2+4)^2-4(\mu+\mu_c)z^2-16\mu\,(z^2+4)^{1/2}\\ &\geq\; 8\mu\big[(z^2+4)^2-z^2-2(z^2+4)^{1/2}\big] \qquad \text{as } \mu_c<\mu\\ &=\; 8\mu\big[(z^2+4)^2-(z^2+4)-2(z^2+4)^{1/2}+4\big] \;=:\; 8\mu\,g(\tilde{x}). \end{aligned}$$

Let $\tilde{x} := z^2+4$. For $4 \leq \tilde{x} \leq \frac{4\mu^2}{(\mu-\mu_c)^2}$ (due to (35), as $z < z_{\text{crit}}$) the function

$$g(\tilde{x}) := \tilde{x}^2 - \tilde{x} - 2\tilde{x}^{1/2} + 4$$

has a unique minimum at $\tilde{x}=1$ and is strictly positive for all $\tilde{x} \geq 0$. This proves $I_7(z) > 0$ on A_4 and with (57) we obtain $\frac{\partial^2 l_4}{\partial z^2}(z,\alpha) \geq 0$. Together with $\frac{\partial^2 l_4}{\partial z \partial \alpha}(z,\alpha) > 0$, $\frac{\partial^2 l_4}{\partial \alpha^2}(z,\alpha) = 0$, this is sufficient to proof the convexity of $l_4(z,\alpha)$ on A_4 for the cone $z \geq 0$, $\alpha \geq 0$.

Now let $\mu < \mu_c$. In order to prove $\frac{\partial^2}{\partial z^2} l_4 \geq 0$ we need to show that

$$I_8(z) := 8\mu\,(z^2+4)^2 - 4(\mu+\mu_c)\,z^2 - 16\mu\,(z^2+4)^{1/2} + 2(\mu-\mu_c)(2\pi-\alpha_2(z))z^3 \geq 0$$

for $0 \leq z \leq 2\sqrt{\mu_c(2\mu-\mu_c)}$. Using $\mu-\mu_c \geq -\mu$ and $-4(\mu+\mu_c)z^2 \geq -12\mu z^2$, we obtain

$$\begin{aligned} I_8(z) \;&\geq 2\mu\big[4(z^2+4)^2-6z^2-8(z^2+4)^{1/2}-(2\pi-\alpha_2(z))z^3\big]\\ &= 2\mu\Big[4z^4-2\pi z^3+\arctan\Big(\frac{z}{2}\Big)z^3+26z^2-8(z^2+4)^{1/2}+64\Big]. \qquad (59) \end{aligned}$$

A straightforward discussion reveals that the right hand side of (59) is strictly positive on A_4, proving with (57) that $\frac{\partial^2 l_4}{\partial z^2}(z,\alpha) \geq 0$ on A_4.

Part (3): Convexity of $l(z,\alpha)$ on $\overline{D} := [0,2]\times[0,2\pi]$.

We write as before $l_i := l_{|A_i}$ for $i \in \{1,2,3,4\}$. The continuity of l on $\Gamma_{ij} := \overline{A_i}\cap\overline{A_j}$ follows at once from the definition (49) of $l_1,\dots,l_4$ and Eqn. (36).

Due to Part (2), l is convex on each A_i. In order for l to be altogether convex, a jump condition of ∇l on Γ_{ij} must be fulfilled. With fixed $(\overline{z},\overline{\alpha})\in\Gamma_{ij}$, letting

$$G_i := \lim_{\substack{(z,\alpha)\to(\overline{z},\overline{\alpha})\\ (z,\alpha)\in \mathrm{int}A_i}} \nabla l_i(z,\alpha), \qquad G_j := \lim_{\substack{(z,\alpha)\to(\overline{z},\overline{\alpha})\\ (z,\alpha)\in \mathrm{int}A_j}} \nabla l_j(z,\alpha),$$

this jump condition at $(\overline{z},\overline{\alpha})$ reads

$$(G_i - G_j)\cdot\vec{n} \geq 0. \tag{60}$$

Here $\vec{n}$ is the normal vector at $(\overline{z},\overline{\alpha})\in\Gamma_{ij}$ pointing from A_i to A_j. In this context we also refer to [2], where general conditions for the convexity of piecewise-defined functions are derived. The results in [2] are not applicable here since the sets A_1, A_3, A_4 are non-convex, cf. Fig. 6. We subsequently check the validity of (60) on each Γ_{ij}.

First we consider $\Gamma_{14} = \{(z,\alpha_2(z))\in\overline{D} \mid z < z_{\mathrm{crit}}\}$. Direct computations yield

$$\frac{\partial l_4}{\partial z}(z,\alpha_2(z)) = \underline{e}'_{\mu,\mu_c}(z) = \frac{2\mu z}{(z^2+4)^{1/2}}\Big((z^2+4)^{1/2}-1\Big) = \frac{\partial l_1}{\partial z}(z,\alpha_2(z)). \tag{61}$$

Because of

$$\frac{\partial l_4}{\partial \alpha}(z,\alpha_2(z)) = 0 = \frac{\partial l_1}{\partial \alpha}(z,\alpha_2(z)), \tag{62}$$

the jump condition (60) holds with equality on Γ_{14}.

We observe that a two-dimensional curve $\Gamma = (x(t),y(t))$ possesses the normal

$$\vec{n}(t) = \frac{1}{(\dot{x}(t)^2+\dot{y}(t)^2)^{1/2}}(-\dot{y}(t),\dot{x}(t)). \tag{63}$$

On $\Gamma_{23} = \{(z,\alpha_1^+(z))\in\overline{D} \mid z \geq z_{\mathrm{crit}}\}$, due to (63), $\vec{n}(z)\sim(-\alpha_1^+(z)',1)$. So, (60) becomes

$$\begin{pmatrix} \frac{2\mu_c^2}{|\mu-\mu_c|}\,\frac{\alpha-2\pi}{(2\pi-\alpha_1^+(z))^2}\alpha_1^+(z)' \\ \frac{2\mu_c^2}{|\mu-\mu_c|}(2\pi-\alpha_1^+(z))^{-1} \end{pmatrix}\cdot\begin{pmatrix} -\alpha_1^+(z)' \\ 1 \end{pmatrix} \geq 0.$$

This is equivalent to

$$\frac{2\mu_c^2}{|\mu-\mu_c|}\Big(\frac{2\pi-\alpha}{(2\pi-\alpha_1^+(z))^2}\,(\alpha_1^+(z)')^2 + \big(2\pi-\alpha_1^+(z)\big)^{-1}\Big) \geq 0. \tag{64}$$

Clearly, (64) is satisfied on $\overline{D}$ proving the validity of (60) on Γ_{23}.

On $\Gamma_{12} = \{(z, \alpha_1^-(z)) \in \overline{D} \mid z \geq z_{\mathrm{crit}}\}$, let $v(z) := \frac{2\mu z - 2f(z)}{4\mu + zf(z)}$ such that $\alpha_1^-(z) = \arctan(v(z))$. Direct computations show that on Γ_{12}

$$\begin{aligned} \frac{\partial l_1}{\partial z}(z,\alpha) - \frac{\partial l_2}{\partial z}(z,\alpha) &= \frac{v(z)}{v(z)^2+1}\Big[(\mu-\mu_c)(zv(z)+2) - 2\mu(v(z)^2+1)^{1/2}\Big], \\ \frac{\partial l_1}{\partial \alpha}(z,\alpha) - \frac{\partial l_2}{\partial \alpha}(z,\alpha) &= \frac{z-2v(z)}{v(z)^2+1}\Big[(\mu-\mu_c)(zv(z)+2) - 2\mu(v(z)^2+1)^{1/2}\Big]. \end{aligned} \tag{65}$$

Due to (63), $\vec{n}(z) = (-\frac{v'(z)}{v(z)^2+1}, 1)$ and the jump condition (60) reads

$$\frac{2\mu(v(z)^2+1)^{1/2} - (\mu-\mu_c)(zv(z)+2)}{v(z)^2+1}\begin{pmatrix} v(z) \\ z-2v(z) \end{pmatrix} \cdot \begin{pmatrix} -\frac{v'(z)}{v(z)^2+1} \\ 1 \end{pmatrix} \geq 0. \tag{66}$$

A straightforward computation shows that

$$2\mu(v(z)^2+1)^{1/2} - (\mu-\mu_c)(zv(z)+2) = 0. \tag{67}$$

As the prefactor in (66) vanishes the jump condition (60) holds with equality on Γ_{12}.

On $\Gamma_{34} = \{(z_{\mathrm{crit}}, \alpha) \in \overline{D} \mid \arctan(\frac{z_{\mathrm{crit}}}{2}) \leq \alpha \leq 2\pi\}$, $\vec{n} = (1,0)^t$, cf. Fig. 6. Furthermore $\alpha_1^+(z_{\mathrm{crit}}) = \alpha_2(z_{\mathrm{crit}}) = \arctan(\frac{z_{\mathrm{crit}}}{2})$ by Eqn. (36). Therefore, (60) becomes

$$\frac{\partial l_4}{\partial z}(z_{\mathrm{crit}}, \alpha) \geq \frac{\partial l_3}{\partial z}(z_{\mathrm{crit}}, \alpha) \quad \text{for } \arctan\Big(\frac{z_{\mathrm{crit}}}{2}\Big) \leq \alpha \leq 2\pi. \tag{68}$$

We find $\frac{\partial l_4}{\partial z}(z_{\mathrm{crit}}, \alpha) = e'(z_{\mathrm{crit}})$ and (68) turns into

$$2\mu\, z_{\mathrm{crit}} - \frac{2\mu\, z_{\mathrm{crit}}}{(z_{\mathrm{crit}}^2+4)^{1/2}} \geq (\mu+\mu_c) z_{\mathrm{crit}}.$$

This simplifies to

$$\mu - \frac{2\mu}{(z_{\mathrm{crit}}^2+4)^{1/2}} \geq \mu_c. \tag{69}$$

Using $z_{\mathrm{crit}}^2 + 4 = \frac{4\mu^2}{(\mu-\mu_c)^2}$ in (69), we get $\mu - (\mu-\mu_c) \geq \mu_c$ and (60) holds on Γ_{34} with equality.

Part (4): $l \leq Q$.

The condition $l \leq Q$ is equivalent to $L \leq W$. The latter is evident since by construction, $L(z,\alpha) = W(z,\alpha)$ in the region where W is convex, while otherwise L is an affine function below W connecting the minimizers of W.

Part (5): $l(z,\alpha)$ is greater or equal any convex function less or equal Q.

By Minkowski's theorem, if $((z,\alpha),s) \in \mathbb{R}^2 \times \mathbb{R}$ is an extreme point (see, e.g., [15, Def. 2.17] for a definition) of $\mathrm{epi}(W^{**})$, then

$$s = W^{**}(z,\alpha) = W(z,\alpha). \tag{70}$$

This implies $W(z,\alpha) = W^{**}(z,\alpha) = l(z,\alpha) - \frac{\mu}{2}|z|^2$ or equivalently $Q(z,\alpha) = l(z,\alpha)$ in $(z, \alpha_1^{\pm}(z))$ if $z \geq z_{\text{crit}}$ and in $(z, \alpha_2(z))$ if $z < z_{\text{crit}}$. Due to the result in [32], the largest convex function l majorized by Q in $\overline{D}$ solves the nonlinear degenerate elliptic PDE

$$T[l](z,\alpha) := \min\Big\{Q(z,\alpha) - l(z,\alpha), \lambda_1[\mathcal{D}^2 l](z,\alpha)\Big\} \ = \ 0, \tag{71}$$

where $\lambda_1[\mathcal{D}^2 l]$ denotes the smallest eigenvalue of the Hessian of l. Due to (71), in the non-contact set $\{l < Q\}$, it holds $\lambda_1[\mathcal{D}^2 l] = 0$ and l must be flat in at least one direction. In the case investigated here, l is flat in the α-direction. On the other hand, the largest underestimator cannot be affine in z-direction because of the strict convexity of $z \mapsto Q(z,\alpha)$. This proves the optimality of $l(z,\alpha)$. □

Remark 4. *We doublechecked the correctness of (44)–(46) with a small MATLAB code that generates a large set of discrete points in* $\mathrm{epi}(Q) \cap ([0,2] \times [0,2\pi])$ *and computes the closed convex hull of this set. Because of*

$$\mathrm{epi}(Q^{**}) = \overline{\mathrm{co}}(\mathrm{epi}(Q)), \tag{72}$$

this computes the epigraph of Q^{**} from which the graph of Q^{**} can be read off. In (72), $\mathrm{epi}(Q)$ *denotes the epigraph of Q and* $\overline{\mathrm{co}(A)}$ *is the closed convex hull of a set A. The MATLAB algorithm is available as supplementary material to this article.*

Fig. 7 shows one example computed by the algorithm and compares its result with the analytic formula given in Lemma 2.

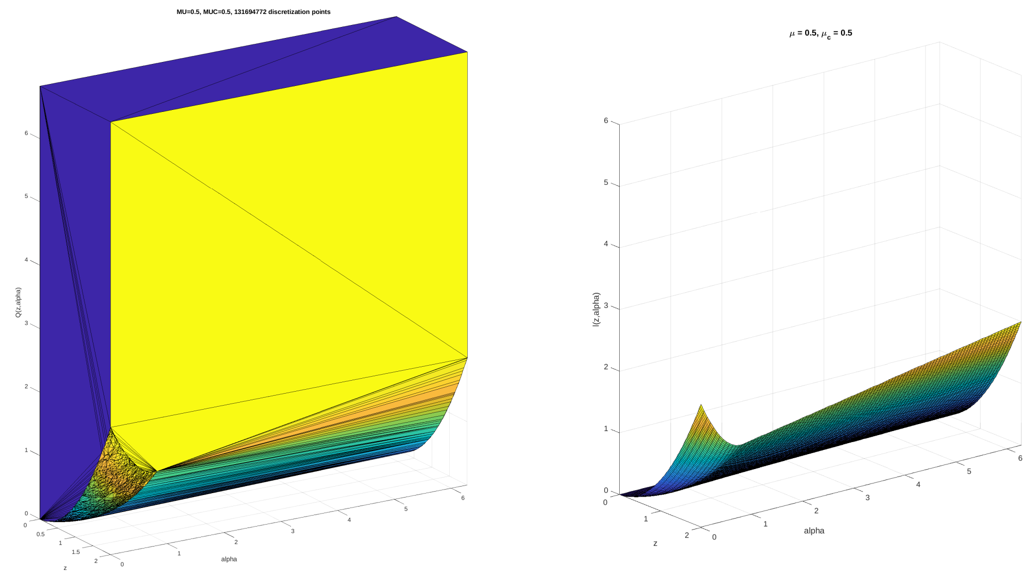

Figure 7: Left: Simplified triangulation of the convexification of epi(Q) for $(z, \alpha) \in [0, 2] \times [0, 2\pi]$ and $\mu = \mu_c = 0.5$ as computed by our algorithm. The lateral and top surfaces are in blue, the color of the front depends on the value of z (e.g. yellow for $z = 2$). Right: Plot of $l(z, \alpha)$ for $(z, \alpha) \in [0, 2] \times [0, 2\pi]$ and $\mu = \mu_c = 0.5$ defined by the right hand side of Eqn. (45), cf. the proof of Lemma 2. In both plots one can identify the region on the bottom left where $Q(z, \alpha) = Q^{**}(z, \alpha) = W(z, \alpha) + \frac{\mu}{2} z^2$.

4. Conclusion

In this paper, the zero-order Gamma-limit of $E(u, \alpha)$ has been computed and the minimizers have been identified. In particular, the results reveal the fine properties of the optimal micro-rotations α forming transition layers in Ω.

The relaxed functional E_0 may also be of interest for numerical simulations. Using E_0 instead of the original Cosserat functional E given by (5) for simulations with a small but finite $L_c > 0$ corresponds to a convexification or homogenization of the problem and may help apart from a very significant speed up to avoid some of the numerical problems encountered in [7, 8, 9].

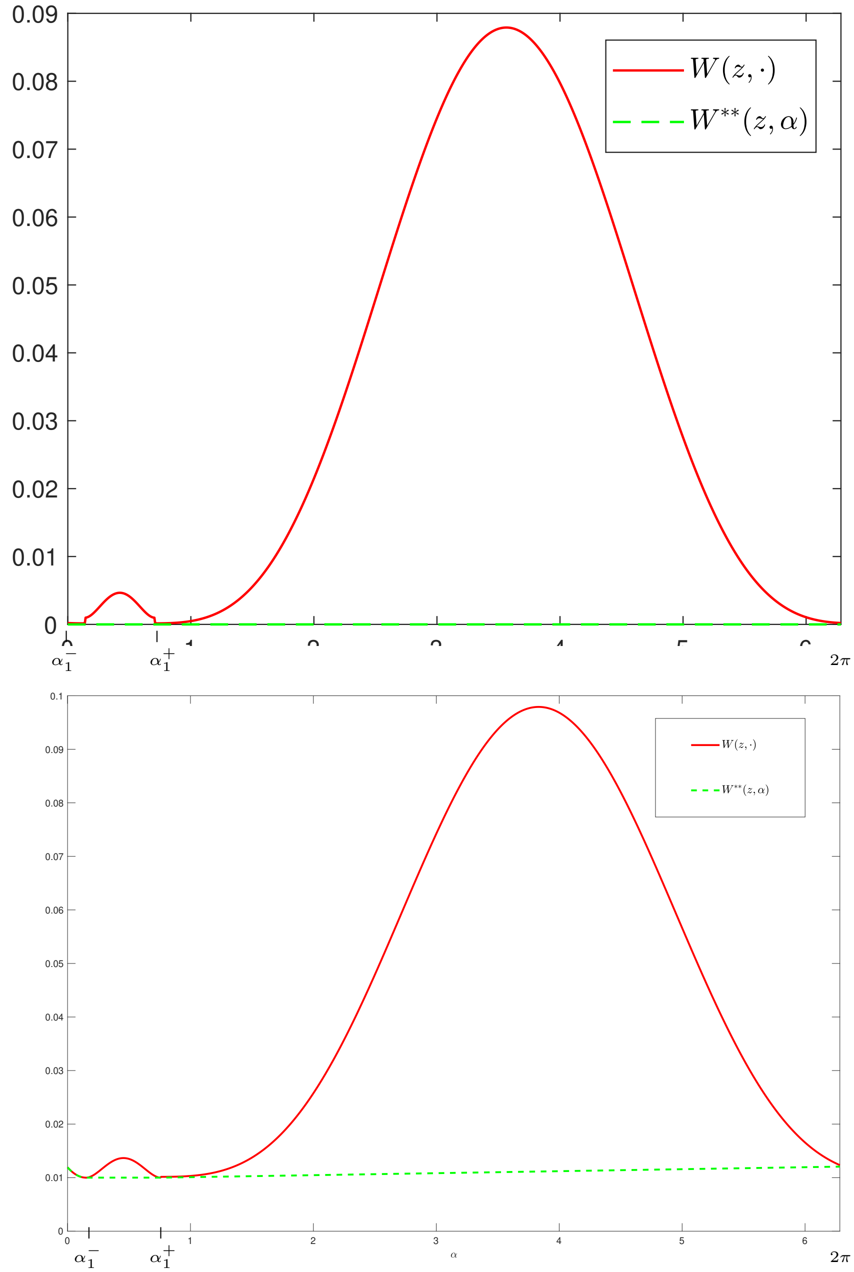

Figure 8: Sketch of the construction of the underestimator $L(z,\alpha)$ of $W(z,\alpha)$ in the proof of Lemma 2 leading to $Q^{**}(z,\alpha)$. Top: The special case (i) with $\mu_c = 0$. Connecting the minima of $W(z,\cdot)$ at $\alpha = \alpha_1^- = 0$, at $\alpha = \alpha_1^+(z)$ and at $\alpha = 2\pi$ with minimal energy 0 yields $L(z,\alpha) \equiv 0$. Bottom: The case (iii), here with $\mu_c < \mu$, for fixed $z \geq z_{\text{crit}}$. For $\alpha \in [0, \alpha_1^-(z))$, $W(z,\cdot)$ is strictly convex. For $\alpha \in [\alpha_1^-(z), \alpha_1^+(z)]$, $L(z,\alpha) \equiv \underline{e}_{\mu,\mu_c}(z) - \frac{\mu}{2}z^2$ is constant, connecting the two minima by a straight line. For $\alpha \in [\alpha_1^+, 2\pi]$, $L(z,\alpha)$ is a slightly increasing affine function, connecting $(\alpha_1^+(z), W(z,\alpha_1^+(z)))$ with $(2\pi, W(z,2\pi))$. In both plots, the double well is strongly exaggerated to better illustrate the principle.

Appendix – Pointwise minimization of E for $L_c = 0$

It is instructive to compare the zero-order Gamma-limit of E_ε, i.e. the results of Proposition 1 and Lemma 2, with the following *pointwise minimization*. Let $\widetilde{E}_0$ be defined by (10) which coincides with E given by Eqn. (5) with $L_c = 0$. For chosen deformation $u \in \mathcal{X}_u$, we denote by $\alpha_{\text{opt}} = \alpha_{\text{opt}}(u')$ a corresponding optimal micro-rotation, i.e. a rotation $\alpha \in \mathcal{X}_a$ that minimizes $\alpha \mapsto E(u, \alpha)$ for fixed u. Plugging in α_{opt} into $\widetilde{E}_0$, we end up with the functional

$$\begin{aligned} E_{\text{opt}}(u) &:= \widetilde{E}_0(u, \alpha_{\text{opt}}(u')) \\ &= \frac{\mu}{2}\int_0^1 |u'|^2 + \big(\sin(\alpha_{\text{opt}})u' - 4\sin^2\big(\frac{\alpha_{\text{opt}}}{2}\big)\big)^2\,\mathrm{d}x \\ &\quad + \frac{\mu_c}{2}\int_0^1 \big(\cos(\alpha_{\text{opt}})u' - 2\sin(\alpha_{\text{opt}})\big)^2\,\mathrm{d}x. \end{aligned} \tag{73}$$

The following proposition computes E_{opt} explicitly for the different regimes.

Proposition 2 (Pointwise minimization of E for $L_c = 0$). *Let E_{opt} be given by (73) and assume $u \in \mathcal{X}_u$. Then it holds*
(i) If $\mu \neq \mu_c$ and $\alpha_1^\pm$ exists:

$$E_{\text{opt}}(u) = \frac{\mu + \mu_c}{2}\int_0^1 |u'|^2\,\mathrm{d}x - \frac{2\mu_c^2}{|\mu - \mu_c|}. \tag{74}$$

(ii) If $\mu = \mu_c$ or ($\mu \neq \mu_c$ and $\alpha_1^\pm$ do not exist):

$$E_{\text{opt}}(u) = \mu\int_0^1 |u'|^2 + 4 - 2\big(|u'|^2 + 4\big)^{1/2}\,\mathrm{d}x. \tag{75}$$

The functional E_{opt} defined by (74) or (75) is convex in u'.

We observe that $\mu_c = 0$ is a special case of (i) for which Eqn. (74) simplifies to

$$E_{\text{opt}}(u) = \frac{\mu}{2}\int_0^1 |u'|^2\,\mathrm{d}x. \tag{76}$$

Proof. Consider the Euler-Lagrange equation w.r.t. α of $\widetilde{E}_0$ defined in (10),

$$0 \;=\; \big(\cos(\alpha)u' - 2\sin(\alpha)\big)\Big[(\mu - \mu_c)\Big(\sin(\alpha)u' - 4\sin^2\big(\frac{\alpha}{2}\big)\Big) - 2\mu_c\Big]. \tag{77}$$

Eqn. (77) states an algebraic relationship between α and u' since $L_c = 0$. Resolving Eqn. (77) leads to the minimizing optimal rotations $\alpha_{\rm opt} = \alpha_{\rm opt}(u')$ summarized in Table 1.

(i) Let $\mu \neq \mu_c$ and $\alpha_1^\pm$ exists. First consider $\mu_c = 0$. The optimal rotations in this case are

$$\alpha_{\rm opt} = \alpha_1^- = 0, \qquad \alpha_{\rm opt}(u') = \alpha_1^+ = 2\arctan\Big(\frac{u'}{2}\Big), \tag{78}$$

cf. Table 1 and Eqn. (33). In both cases, $\big(\sin(\alpha_{\rm opt})u' - 4\sin^2(\alpha_{\rm opt}/2)\big)^2 = 0$, and (73) at once simplifies to (76).

Now consider the case $\mu_c > 0$.

With $f := \big((|u'|^2+4)(\mu-\mu_c)^2 - 4\mu^2\big)^{1/2}$, cf. Eqn. (30), the two optimal rotations are

$$\alpha_{\rm opt}(u') = \alpha_1^+ = \arctan\Big(\frac{\mu u' + f}{2\mu - \frac{u'}{2}f}\Big), \qquad \alpha_{\rm opt}(u') = \alpha_1^- = \arctan\Big(\frac{\mu u' - f}{2\mu + \frac{u'}{2}f}\Big).$$

By direct inspection, we find

$$\begin{aligned}\sin(\alpha_1^-)u' + 2\cos(\alpha_1^-) &= \frac{2\mu}{\mu-\mu_c}, \qquad &\cos(\alpha_1^-)u' - 2\sin(\alpha_1^-) &= \frac{f}{\mu-\mu_c},\\ \sin(\alpha_1^+)u' + 2\cos(\alpha_1^+) &= \frac{2\mu}{\mu-\mu_c}, \qquad &\cos(\alpha_1^+)u' - 2\sin(\alpha_1^+) &= \frac{-f}{\mu-\mu_c}.\end{aligned} \tag{79}$$

Plugging these identities into (73), we obtain for both choices of $\alpha_{\rm opt}$

$$\begin{aligned} E_{\rm opt}(u) &= \frac{\mu}{2}\int_0^1 |u'|^2 + \Big(\frac{2\mu}{\mu-\mu_c} - 2\Big)^2 {\rm d}x + \frac{\mu_c}{2}\int_0^1 \frac{f^2}{(\mu-\mu_c)^2}\,{\rm d}x \\ &= \frac{\mu}{2}\int_0^1 |u'|^2\,{\rm d}x + \frac{2\mu\mu_c^2}{(\mu-\mu_c)^2} + \frac{\mu_c}{2}\int_0^1 \frac{(|u'|^2+4)(\mu-\mu_c)^2 - 4\mu^2}{(\mu-\mu_c)^2}\,{\rm d}x \\ &= \frac{\mu+\mu_c}{2}\int_0^1 |u'|^2\,{\rm d}x + \frac{2\mu\mu_c^2}{(\mu-\mu_c)^2} + \frac{\mu_c}{2}\,\frac{4\mu_c^2 - 8\mu\mu_c}{(\mu-\mu_c)^2}. \end{aligned} \tag{80}$$

This simplifies to (74).

(ii) Let $\mu = \mu_c$ or ($\mu \neq \mu_c$ and $\alpha_1^\pm$ do not exist). The unique optimal rotation in this case is $\alpha_{\rm opt}(u') = \alpha_2 = \arctan\big(\frac{u'}{2}\big)$. For $t \in \mathbb{R}$ we remark the identities

$$\cos(\arctan(t)) \;=\; \frac{1}{(t^2+1)^{1/2}}, \qquad \sin(\arctan(t)) \;=\; \frac{t}{(t^2+1)^{1/2}}. \tag{81}$$

With (81), direct inspection yields $\sin(\alpha_2) = \frac{u'}{(|u'|^2+4)^{1/2}}$, $\cos(\alpha_2) = \frac{2}{(|u'|^2+4)^{1/2}}$ such that

$$\begin{aligned} &\cos(\alpha_2)u' - 2\sin(\alpha_2) = 0, \\ &\big(\sin(\alpha_2)u' + 2\cos(\alpha_2) - 2\big)^2 = \Big(\frac{|u'|^2+4}{(|u'|^2+4)^{1/2}} - 2\Big)^2 \;=\; |u'|^2 + 8 - 4\big(|u'|^2+4\big)^{1/2}. \end{aligned} \tag{82}$$

Using the identity $-4\sin^2\big(\frac{\alpha_{\rm opt}}{2}\big) = 2\cos(\alpha_{\rm opt}) - 2$, this shows for case (ii)

$$E_{\rm opt}(u) = \frac{\mu}{2}\int_0^1 |u'|^2 + \big(\sin(\alpha_2)u' + 2\cos(\alpha_2) - 2\big)^2\,{\rm d}x = \mu\int_0^1 |u'|^2 + 4 - 2\big(|u'|^2+4\big)^{1/2}\,{\rm d}x$$

which is (75).

The convexity of $E_{\rm opt}$ given by Eqn. (74) is evident. But also Eqn. (75) defines a convex functional in $z = u'$, even though it may first not appear so. Indeed, introducing $g : \mathbb{R} \to \mathbb{R}$,

$$g(z) := z^2 + 4 - 2\big(z^2+4\big)^{1/2},$$

a direct computation yields $g'(z) = 2z - 2z\big(z^2+4\big)^{-1/2}$ and

$$g''(z) = 2 + \frac{2z^2}{(z^2+4)^{3/2}} - \frac{2}{(z^2+4)^{1/2}} \;=\; \frac{2(z^2+4)^{3/2} - 8}{(z^2+4)^{3/2}} \;>\; 0.$$

This is the convexity of g and hence of $E_{\rm opt}$ in u' as defined by Eqn. (75). □

Remark 5. *When $\mu_c = 0$, $E_{\rm opt}(u)$ coincides with $E_0 := \Gamma\text{–}\lim_{\varepsilon\searrow 0} E_\varepsilon$ computed in Prop. 2 and Lemma 2. For all other cases of Proposition 2, $E_{\rm opt}$ differs from the Gamma-limit E_0. This underlines the critical role of the Cosserat couple modulus μ_c in the modelling.*

Remark 6. *A direct minimization analogous to (73) is also possible in three space dimensions for $\widetilde{E}_{3D}$, cf. Eqn. (11). In [28, 19, 20], the optimal rotations are computed, see also [7, 9] for numerical considerations. However, for $\mu_c \geq \mu$ it is known, [29], that the resulting functional*

$$\int_{\widehat{\Omega}} \mu\,{\rm dist}^2\big(F, {\rm SO}(n)\big) + \frac{\lambda}{4}\Big[(\det \overline{U} - 1)^2 + \Big(\frac{1}{\det \overline{U}} - 1\Big)^2\Big]\,{\rm d}x$$

is not rank-one convex due to the dist*-function. The computation of the quasi-convex hull w.r.t. deformations in* $\mathrm{GL}^+(2)$ *in this case can be found in [21].*

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