# Dissipation distances in multiplicative elastoplasticity

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**Abstract.** We study finite-strain elastoplasticity in a new formulation proposed in [Mie02b,CHM02,Mie02a]. This theory does not need smoothness and is based on energy minimization techniques. In particular, it gives rise to robust algorithms. It is based on two scalar constitutive functions: an elastic potential and a dissipation potential which give rise to an energy functional and a dissipation distance.

Here we study these dissipation distances in some detail and present situations where they are quite explicitly available. These include isotropic plasticity of Prandtl-Reuß type and examples from two-dimensional single-crystal plasticity. We put special emphasis on the geometric nonlinearities arising from the underlying matrix groups which lead to optimization problems on Lie groups.

#### 1 Introduction

In the recent papers [Mie02b,CHM02,Mie02a] a new energetic formulation for finite strain elasto–plasticity was proposed. It is based on computational algorithms used in engineering, cf. [OR99,ORS00,HH02,ML01,MSL01]. This theory is based on the elastic potential  $\psi$  and the dissipation potential  $\Delta$  as the underlying constitutive functions:

$$\psi = \widehat{\psi}(\mathbf{F}, \mathbf{P}, p)$$
 and  $\Delta = \widehat{\Delta}(\mathbf{P}, p, \dot{\mathbf{P}}, \dot{p}) \geq 0$ 

where  $\mathbf{F} = \mathbf{D}\boldsymbol{\varphi} = \mathbf{F}_{\mathrm{el}}\mathbf{F}_{\mathrm{pl}}$  is the total deformation gradient,  $\mathbf{P} = \mathbf{F}_{\mathrm{pl}}^{-1}$  the inverse plastic deformation and  $p \in \mathbb{R}^m$  denote the hardening variables. The plastic tensor  $\mathbf{P}$  is usually assumed to have determinant 1, i.e.  $\mathbf{P}$  is an element of the special linear group  $\mathrm{SL}(d) = \{ \mathbf{P} \in \mathbb{R}^{d \times d} \mid \det \mathbf{P} = 1 \}$ . Consequently,  $\widehat{\Delta}$  is defined on the tangent bundle of the manifold  $\mathrm{SL}(d) \times \mathbb{R}^m$ . The axiom of plastic indifference implies

$$\widehat{\psi}(\mathbf{F},\mathbf{P},p) = \widetilde{\psi}(\mathbf{F}\mathbf{P},p), \qquad \widehat{\Delta}(\mathbf{P},p,\dot{\mathbf{P}},\dot{p}) = \widetilde{\Delta}(p,\mathbf{P}^{-1}\dot{\mathbf{P}},\dot{p}).$$

This means that the underlying mathematical structure is that of the Lie group SL(d), a fact which was first emphasized in [Mie02b]. Rate-independency is expressed by the fact, that  $\widehat{\Delta}$  is homogeneous of degree 1 in the rate  $(\dot{\mathbf{P}}, \dot{p})$ , see (Sy3) in Section 2.1.

The full global energetic formulation relies heavily on the (global) distance  $\widehat{D}(x,\cdot,\cdot)$ , called dissipation distance, which is generated via the infinitesimal metric  $\widehat{\Delta}(x,\cdot,\cdot)$  on  $\mathrm{SL}(d)\times\mathbb{R}^m$  as follows: the distance  $\widehat{D}((\mathbf{P}_0,p_0),(\mathbf{P}_1,p_1))$  is the infimum of the dissipation  $\int_0^1 \widehat{\Delta}(\mathbf{P}(s),p(s),\dot{\mathbf{P}}(s),\dot{p}(s))\,\mathrm{d}s$  over all paths  $(\mathbf{P},p)\in\mathrm{C}^1([0,1],\mathrm{SL}(d)\times\mathbb{R}^m)$  with  $(\mathbf{P}(j),p(j))=(\mathbf{P}_j,p_j)$  for j=0,1. Consider now a body  $\Omega\subset\mathbb{R}^d$ , a deformation  $\varphi:\Omega\mapsto\mathbb{R}^d$  as well as internal states  $(\mathbf{P}_j,p_j):\Omega\mapsto\mathrm{SL}(d)\times\mathbb{R}^n$ , then integration over  $\Omega$  gives the total energies

$$\mathcal{E}(t, \boldsymbol{\varphi}, \mathbf{P}, p) = \int_{\Omega} \widehat{\psi}(\mathbf{D}\boldsymbol{\varphi}(x), \mathbf{P}(x), p(x)) \, \mathrm{d}x - \langle \ell(t), \boldsymbol{\varphi} \rangle,$$

$$\mathcal{D}((\mathbf{P}_0, p_0), (\mathbf{P}_1, p_1)) = \int_{\Omega} \widehat{D}((\mathbf{P}_0(x), p_0(x)), (\mathbf{P}_1(x), p_1(x))) \, \mathrm{d}x,$$

where  $\ell(t)$  denotes the external loading depending on the process time  $t \in [0,T]$ . A triple  $(\varphi, \mathbf{P}, p) : [0,T] \times \Omega \mapsto \mathbb{R}^d \times \mathrm{SL}(d) \times \mathbb{R}^m$  is called a **solution process** if it satisfies the following stability condition (S) and the energy inequality (E):

(S) [Stability] For all  $t \in [0,T]$  and all comparison states  $(\widetilde{\varphi}, \widetilde{\mathbf{P}}, \widetilde{p})$  we have

$$\mathcal{E}(t, \varphi(t), \mathbf{P}(t), p(t)) \leq \mathcal{E}(t, \widetilde{\varphi}, \widetilde{\mathbf{P}}, \widetilde{p}) + \mathcal{D}((\mathbf{P}(t), p(t)), (\widetilde{\mathbf{P}}, \widetilde{p})).$$

(E) [Energy inequality] For all  $0 \le t_1 < t_2 \le T$  we have

$$\begin{split} & \mathcal{E}(t_2, \boldsymbol{\varphi}(t_2), \mathbf{P}(t_2), p(t_2)) + \operatorname{Diss}((\mathbf{P}, p); [t_1, t_2]) \\ & \leq & \mathcal{E}(t_1, \boldsymbol{\varphi}(t_1), \mathbf{P}(t_1), p(t_1)) - \int_{t_1}^{t_2} \langle \dot{\boldsymbol{\ell}}(s), \boldsymbol{\varphi}(s) \rangle \, \mathrm{d}s, \end{split}$$

where 
$$\operatorname{Diss}((\mathbf{P},p);[t_1,t_2]) = \int_{t_1}^{t_2} \int_{\Omega} \widehat{\Delta}(x,(\mathbf{P},p),(\dot{\mathbf{P}},\dot{p})) dx ds.$$

Note that (S) & (E) characterize the process completely and that this formulation does not involve any derivatives, neither of  $\mathbf{F} = \mathrm{D} \boldsymbol{\varphi}$ ,  $\mathbf{P}$  and p (with respect to t or x) nor of the constitutive functions  $\widehat{\psi}$  and  $\widehat{\Delta}$ . It is shown in [Mie02a] that this formulation is consistent with the usual flow rules of finite plasticity if the solution of (S) & (E) is sufficiently smooth. In fact, using the Legendre transform there is a one-to-one correspondence between  $\widehat{\Delta}$  and an associative flow rule for a suitable yield surface.

The purpose of this work is the investigation of the global **dissipation distance**  $\widehat{D}$  in cases when we have no hardening or just a scalar variable measuring the total hardening. The major object studied here is a left–invariant metric  $\widehat{D}: \mathrm{SL}(d) \times \mathrm{SL}(d) \to [0,\infty]$  generated by  $\widetilde{\Delta}: \mathfrak{sl}(d) \to [0,\infty]$  via

$$\widehat{D}(\mathbf{P}_0, \mathbf{P}_1) := \inf \left\{ \int_0^1 \widetilde{\Delta}(\mathbf{P}(t)^{-1}\dot{\mathbf{P}}(t)) \, \mathrm{d}t \mid \mathbf{P}(\cdot) \in \mathrm{C}^1([0, 1], \mathrm{SL}(d)), \\ \mathbf{P}(0) = \mathbf{P}_0, \ \mathbf{P}(1) = \mathbf{P}_1 \right\}.$$

In this work we only investigate the two-dimensional case, so we consider SL(2), the three-dimensional Lie group of  $2\times 2$  matrices with determinant 1. A few results for the three-dimensional case are given in [Mie02b].

For the isotropic case with d=2 we derive an explicit formula for  $\widehat{D}$ . This case is characterized by

$$\widetilde{\Delta}(\boldsymbol{\xi}) = \left(\frac{\alpha}{4}|\boldsymbol{\xi} + \boldsymbol{\xi}^{\mathsf{T}}|^2 + \frac{\beta}{4}|\boldsymbol{\xi} - \boldsymbol{\xi}^{\mathsf{T}}|^2\right)^{1/2}, \text{ where } |\boldsymbol{\eta}|^2 = \operatorname{trace}(\boldsymbol{\eta}^{\mathsf{T}}\boldsymbol{\eta})$$

and  $\alpha > 0$ ,  $\beta \in [0, \infty]$  are material parameters. In this case  $\widehat{D}(\mathbf{P}_0, \mathbf{P}_1)$  can be shown to depend solely on the two invariants of  $\mathbf{Q} = \mathbf{P}_0^{-1} \mathbf{P}_1$ , i.e., the trace and the norm of  $\mathbf{Q}$ .

Second we report on results for the case of single crystal plasticity where  $\widetilde{\Delta}$  is characterized via slip systems  $\mathbf{S}^{\alpha}$ ,  $\alpha = 1, \ldots, m$  as follows

$$\widetilde{\Delta}(\boldsymbol{\xi}) = \min \left\{ \sum_{\alpha=1}^{m} \kappa_{\alpha} \gamma_{\alpha} \mid \boldsymbol{\xi} = \sum_{\alpha=1}^{m} \gamma_{\alpha} \mathbf{S}^{\alpha} \text{ with } \gamma_{\alpha} \geq 0 \right\},\,$$

with the usual convention that the minimum is  $+\infty$  if the set is empty. These cases lead to functions  $\widetilde{\Delta}$  which are piecewise linear. As a consequence one has to expect that geodesic curves which minimize the dissipation distance have corners. Physically these corners correspond to switches between different slip systems.

The case of a square lattice leads to the four slip systems  $\pm \mathbf{S}^1 = \pm \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$  and  $\pm \mathbf{S}^2 = \pm \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ , which is analyzed in detail in [Mit02a]. It is shown that for all geodesic curves  $\mathbf{P} \colon [0,1] \to \mathrm{SL}(2)$  the invariant rate  $\boldsymbol{\xi}(t) = \mathbf{P}(t)^{-1}\dot{\mathbf{P}}(t)$  is piecewise constant and takes values only in  $\{\pm \mathbf{S}^1, \pm \mathbf{S}^2, \pm \frac{1}{2}(\mathbf{S}^1 + \mathbf{S}^2)\}$ . Moreover, the number of switches can be bounded from above by 5.

As is shown in [Mit02a], one easily obtains the solution for a parallelogram lattice from the solution for the square lattice. We also address the case of a hexagonal lattice where N=6 slip systems are present.

Finally we conclude with the calculation of the dissipation distance in the case of a scalar hardening variable.

# 2 Elastoplasticity with hardening parameters

#### 2.1 Constitutive laws

Multiplicative elastoplasticity uses the split  $\mathbf{F} = \mathbf{D}\boldsymbol{\varphi} = \mathbf{F}_{el}\mathbf{F}_{pl}$ , where  $\mathbf{F}_{pl}$  is an internal variable which is assumed to be generated by movements of dislocations and is such that it maps the crystallographic lattice onto itself. Only the remainder  $\mathbf{F}_{el} = \mathbf{F}\mathbf{F}_{pl}^{-1}$  is the part which accounts for elastic energy and stresses. To simplify notation we introduce  $\mathbf{P} = \mathbf{F}_{pl}^{-1}$  as an internal variable together with suitable hardening parameters  $p \in \mathbb{R}^m$ , i.e.

$$z = (\mathbf{P}, p) \in \mathfrak{G} \times \mathbb{R}^m$$
, with  $\mathfrak{G} \subset \mathrm{GL}_+(\mathbb{R}^d)$ .

Here  $\mathfrak{G}$  is a Lie group contained in  $\mathrm{GL}_+(\mathbb{R}^d)$  which might be different from model to model. We let  $\mathfrak{g}$  denote the associated Lie algebra. Typically one chooses  $\mathfrak{G}=\mathrm{SL}(\mathbb{R}^d)=\{\,\mathbf{F}\mid \det\mathbf{F}=1\,\}$ . However,  $\mathfrak{G}=\mathrm{GL}_+(\mathbb{R}^d)$  or, if only one slip system with  $|\mathbf{n}|=|\mathbf{d}|=1$  and  $\mathbf{n}\cdot\mathbf{d}=0$  is active,  $\mathfrak{G}=\{\,\mathbf{I}+\alpha\mathbf{d}\otimes\mathbf{n}\,|\,\alpha\in\mathbb{R}\,\}$  might also be suitable.

The hardening parameters can include isotropic or kinematic hardening, see [Mie02a] and below.

For the constitutive function  $\widehat{\psi}$  and  $\widehat{\Delta}$  we now specify the associated symmetry conditions. They involve the material symmetry group  $\mathfrak{S} \subset \mathrm{SO}(\mathbb{R}^d)$  and they are supposed to hold true for all  $(x,\mathbf{F},\mathbf{P},p)\in\Omega\times\mathrm{GL}_+(\mathbb{R}^d)\times\mathfrak{G}\times\mathbb{R}^m$ :

# (Sy1) Objectivity (frame indifference):

$$\widehat{\psi}(x, \mathbf{RF}, \mathbf{P}, p) = \widehat{\psi}(x, \mathbf{F}, \mathbf{P}, p)$$
 for all  $\mathbf{R} \in SO(3)$ ;

(Sy2) Plastic indifference:

$$\widehat{\psi}(x, \mathbf{F}\mathbf{G}^{-1}, \mathbf{G}\mathbf{P}, p) = \widehat{\psi}(x, \mathbf{F}, \mathbf{P}, p)$$
 and  $\widehat{\Delta}(x, \mathbf{G}\mathbf{P}, p, \mathbf{G}\dot{\mathbf{P}}, \dot{p}) = \widehat{\Delta}(x, \mathbf{P}, p, \dot{\mathbf{P}}, \dot{p})$  for all  $\mathbf{G} \in \mathfrak{G}$ ;

(Sy3) Rate independency:

$$\widehat{\Delta}(x, \mathbf{P}, p, \alpha \dot{\mathbf{P}}, \alpha \dot{p}) = \alpha \widehat{\Delta}(x, \mathbf{P}, p, \dot{\mathbf{P}}, \dot{p}) \text{ for } \alpha \geq 0;$$

(Sy4) Material symmetry:

$$\begin{split} \widehat{\psi}(x,\mathbf{F},\mathbf{PS},\tau_{\mathbf{S}}p) &= \widehat{\psi}(x,\mathbf{F},\mathbf{P},p) \text{ and } \\ \widehat{\Delta}(x,\mathbf{PS},\tau_{\mathbf{S}}p,\dot{\mathbf{PS}},\tau_{\mathbf{S}}\dot{p}) &= \widehat{\Delta}(x,\mathbf{P},p,\dot{\mathbf{P}},\dot{p}) \text{ for all } \mathbf{S} \in \mathfrak{S}. \end{split}$$

Here  $\tau_{\mathbf{S}} \in \mathbb{R}^{m \times m}$  denotes a linear representation of the material symmetry group  $\mathfrak{S}$  on the hardening parameters in  $\mathbb{R}^m$ . It satisfies  $\tau_{\mathbf{S}_1\mathbf{S}_2} = \tau_{\mathbf{S}_2}\tau_{\mathbf{S}_1}$ .

The special assumption for elastoplasticity is the "plastic indifference" (Sy2) which leads to the multiplicative split in  $\widehat{\psi}$  as well as to the correct time rates in the flow rules. We find

$$\widehat{\psi}(x,\mathbf{F},\mathbf{P},p) = \widetilde{\psi}(x,\mathbf{FP},p), \qquad \widehat{\Delta}(x,\mathbf{P},p,\dot{\mathbf{P}},p) = \widetilde{\Delta}(x,p,\mathbf{P}^{-1}\dot{\mathbf{P}},\dot{p}). \quad (1)$$

The consequence of the other symmetries will be studied along with the examples treated below.

### 2.2 Associative flow rules

We will not need the associated flow rules in order to study the energetic formulation of elastoplasticity. However, they give some insight into the underlying structures. In particular, they are very helpful in finding the paths which minimize the dissipation distance between two points. This minimization is closely related to the Pontrjagin Maximum Principle (PMP), which

uses the dual stress variables in the same way as the flow rules in elastoplasticity. We define the thermodynamically conjugate variables

$$\begin{split} \mathbf{Q} &= -\tfrac{\partial}{\partial \mathbf{P}} \widehat{\psi}(x, \mathbf{F}, \mathbf{P}, p) = -\mathbf{F}^\mathsf{T} \tfrac{\partial}{\partial \mathbf{F}_{\mathrm{el}}} \widetilde{\psi}(x, \mathbf{F} \mathbf{P}, p) \in \mathrm{T}^*_{\mathbf{P}} \mathfrak{G} = \mathbf{P}^{-\mathsf{T}} \mathfrak{g}^* \subset \mathbb{R}^{d \times d}, \\ \mathbf{q} &= -\tfrac{\partial}{\partial p} \widehat{\psi}(x, \mathbf{F}, \mathbf{P}, p) = -\tfrac{\partial}{\partial p} \widetilde{\psi}(x, \mathbf{F} \mathbf{P}, p) \in \mathbb{R}^m_*. \end{split}$$

Here  $\mathfrak{g}^*$  denotes the dual Lie algebra which is the set of linear mappings from  $\mathfrak{g}$  into  $\mathbb{R}$  and similarly  $\mathbb{R}^m_*$  denotes the dual space of  $\mathbb{R}^m$ . This notation makes the distinction between the primal internal variables  $(\mathbf{P},p) \in \mathfrak{G} \times \mathbb{R}^m$  and the dual (thermodynamically conjugate) variables  $(\mathbf{P}^\mathsf{T}\mathbf{Q},q) \in \mathfrak{g}^* \times \mathbb{R}^m_*$  more transparent.

The elastic domain  $\mathbb{Q}(x, \mathbf{P}, p)$  associated with  $\widehat{\Delta}(x, \mathbf{P}, \mathbf{p}, \cdot, \cdot)$  is the set of all thermodynamic forces  $(\mathbf{Q}, q)$  which are not large enough to overcome the dissipational friction:

$$\begin{split} \mathbb{Q}(x,\mathbf{P},p) &= [\partial_{(\dot{\mathbf{P}},\dot{p})} \widehat{\Delta}(x,\mathbf{P},p,\cdot,\cdot)](\mathbf{0},0) \\ &= \{\, (\mathbf{Q},q) \mid \mathbf{Q} : \mathbf{V} + q \cdot v \leq \widehat{\Delta}(x,\mathbf{P},p,\mathbf{V},v) \text{ for all } (\mathbf{V},v) \in \mathrm{T}_{\mathbf{P}} \mathfrak{G} \times \mathbb{R}^m \,\}. \end{split}$$

Using (Sy2) and the Lie group structure implying  $T_{\mathbf{P}}\mathfrak{G} = \mathbf{P}\mathfrak{g}$  leads to

$$\mathbb{Q}(x, \mathbf{P}, p) = \{ (\mathbf{Q}, q) \mid \mathbf{Q}: (\mathbf{P}\boldsymbol{\xi}) + q \cdot v \leq \widetilde{\Delta}(x, p, \boldsymbol{\xi}, v) \text{ for all } (\boldsymbol{\xi}, v) \in \mathfrak{g} \times \mathbb{R}^m \}$$
$$= \{ (\mathbf{Q}, q) \mid (\mathbf{P}^\mathsf{T} \mathbf{Q}, q) \in [\partial_{(\boldsymbol{\xi}, v)} \widetilde{\Delta}(x, p, \cdot)] (\mathbf{0}, 0) \} \subset \mathrm{T}^*_{\mathbf{P}} \mathfrak{G} \times \mathbb{R}^m_*.$$

Defining 
$$\widetilde{\mathbb{Q}}(x,p) = \mathbb{Q}(x,1,p) = [\partial_{(\xi,\dot{p})}\widetilde{\Delta}(x,p,\cdot,\cdot)](\mathbf{0},0) \subset \mathfrak{g}^* \times \mathbb{R}^m_*$$
 we find

$$(\mathbf{Q}, q) \in \mathbb{Q}(\mathbf{P}, p) \iff (\mathbf{P}^\mathsf{T}\mathbf{Q}, q) \in \widetilde{\mathbb{Q}}(p).$$
 (2)

The plastically indifferent objects  $\widetilde{\Delta}(p,\cdot,\cdot):\mathfrak{g}\times\mathbb{R}^m\mapsto [0,\infty]$  and  $\widetilde{\mathbb{Q}}(p)\subset \mathfrak{g}^*\times\mathbb{R}^m_*$  are in one–to–one correspondence to each other. On the one hand we have  $\widetilde{\mathbb{Q}}(p)=[\partial_{(\boldsymbol{\xi},\dot{p})}\widetilde{\Delta}(p,\cdot,\cdot)](\mathbf{0},0)$ . On the other hand, for given convex  $\widetilde{\mathbb{Q}}(p)$  the function  $\widetilde{\Delta}(p,\cdot)$  is obtained by Legendre transformation of  $\mathcal{X}_{\widetilde{\mathbb{Q}}(p)}$ , i.e.

$$\widetilde{\Delta}(p,\boldsymbol{\xi},v) = \sup_{(\boldsymbol{\eta},q) \in \widetilde{\mathbb{Q}}(p)} (\boldsymbol{\eta}:\boldsymbol{\xi}+v\cdot q) = \sup_{(\boldsymbol{\eta},q) \in \mathfrak{g}^* \times \mathbb{R}^m_*} [\boldsymbol{\eta}:\boldsymbol{\xi}+v\cdot q - \mathcal{X}_{\widetilde{\mathbb{Q}}(p)}(\boldsymbol{\eta},q)]. \quad (3)$$

The flow rule in the thermodynamically conjugate space now takes the form  $(\mathbf{Q},q) \in [\partial_{(\dot{\mathbf{P}},\dot{p})}\widehat{\Delta}(\mathbf{P},p,\cdot,\cdot)](\dot{\mathbf{P}},\dot{p})$ . Using the above transformation for  $\mathbf{P}$  this is equivalent to

$$(\mathbf{P}^{\mathsf{T}}\mathbf{Q}, q) \in [\partial_{(\boldsymbol{\xi}, \dot{p})} \widetilde{\Delta}(p, \cdot, \cdot)] (\mathbf{P}^{-1}\dot{\mathbf{P}}, \dot{p}) \subset \mathfrak{g}^* \times \mathbb{R}_*^m.$$
(4)

Via the Legendre transform we obtain the formulation in the internal variable space:

$$(\mathbf{P}^{-1}\dot{\mathbf{P}},\dot{p}) \in \partial \mathcal{X}_{\widetilde{\mathbb{Q}}(x,p)}(\mathbf{P}^{\mathsf{T}}\mathbf{Q},q) = N_{(\mathbf{P}^{\mathsf{T}}\mathbf{Q},q)}\widetilde{\mathbb{Q}}(x,p) \subset \mathfrak{g} \times \mathbb{R}^{m}, \qquad (4a)$$

where  $N_zC$  denotes the outer normal cone at z to the convex set C. This is the well–known associative flow rule of multiplicative elastoplasticity. It contains the "plastically indifferent" plastic rate  $\mathbf{P}^{-1}\dot{\mathbf{P}}$  as well as the "plastically indifferent" conjugate force  $\mathbf{P}^{\mathsf{T}}\mathbf{Q} = -\mathbf{F}_{\mathrm{el}}^{\mathsf{T}}\frac{\partial}{\partial \mathbf{F}_{\mathrm{el}}}\widetilde{\psi}(x,\mathbf{F}_{\mathrm{el}},p)$ .

# 3 Dissipation distances in the case without hardening

To facilitate the subsequent discussion we first consider the case without hardening, so  $\Delta = \widehat{\Delta}(\mathbf{P}, \dot{\mathbf{P}}) = \widetilde{\Delta}(\mathbf{P}^{-1}\dot{\mathbf{P}})$  is defined via a norm-like function  $\widetilde{\Delta}: \mathfrak{g} \mapsto [0, \infty]$ . This situation is discussed in [Mie02b] in some detail. The dissipation distance satisfies

$$\widehat{D}(\mathbf{P}_0, \mathbf{P}_1) = \widehat{D}(\mathbf{1}, \mathbf{P}_0^{-1} \mathbf{P}_1) =: \widetilde{D}(\mathbf{P}_0^{-1} \mathbf{P}_1),$$

and  $\widetilde{D} \colon \mathfrak{G} \mapsto [0, \infty]$  satisfies  $\widetilde{D}(\mathbf{1} + \varepsilon \boldsymbol{\xi}) = \varepsilon \widetilde{\Delta}(\boldsymbol{\xi}) + O(\varepsilon^2)$  for  $\varepsilon \to 0$ . By definition,  $\widetilde{D}(\mathbf{e}^{\boldsymbol{\xi}}) \leq \widetilde{\Delta}(\boldsymbol{\xi})$  for all  $\boldsymbol{\xi} \in \mathfrak{g}$ . Hence for  $\mathbf{P} = \mathbf{e}^{\boldsymbol{\xi}_1} \cdot \ldots \cdot \mathbf{e}^{\boldsymbol{\xi}_k}$  the triangle inequality yields the estimate  $\widetilde{D}(\mathbf{P}) \leq \sum_{j=1}^k \widetilde{\Delta}(\boldsymbol{\xi}_j)$ . It is important to observe that, in general,  $\widetilde{D}(\mathbf{e}^{\boldsymbol{\xi}}) < \widetilde{\Delta}(\boldsymbol{\xi})$  which indicates that the matrix exponential curves  $t \mapsto \mathbf{e}^{t\boldsymbol{\xi}}$  are **not** the paths of minimal dissipation.

As the dissipation distance is defined via a variational problem, its computation may be fairly complicated. For practical purposes one would like to know situations where  $\widehat{D}$  is available at reasonable computational cost. We will present several such cases, in particular in the case of single crystal plasticity.

The definition of the dissipation distance  $\widehat{D}$  still contains some redundancy because we assume rate independence (Sy3). A simple reparametrization argument shows that it suffices to consider only curves  $\mathbf{P} \colon [0,1] \to \mathfrak{G}$  for which  $\widetilde{\Delta}(\mathbf{P}^{-1}\dot{\mathbf{P}})$  is constant. Therefore, if we set  $\mathbb{U} = \{ \boldsymbol{\xi} \in \mathfrak{g} \mid \widetilde{\Delta}(\boldsymbol{\xi}) \leq 1 \}$ , we immediately obtain the following characterization:

$$\widehat{D}(\mathbf{P}_0,\mathbf{P}_1) = \inf \left\{ T > 0 \mid \text{ there exists } \mathbf{P} \in C^1([0,T],\mathfrak{G}) \text{ such that } \right\}.$$

$$\mathbf{P}^{-1}\dot{\mathbf{P}} \in \mathbb{U}, \ \mathbf{P}(0) = \mathbf{P}_0, \ \mathbf{P}(T) = \mathbf{P}_1$$

Thus  $\widehat{D}$  is characterized via the solution of a time-optimal control problem. The underlying ODE is  $\dot{\mathbf{P}}(t) = \mathbf{P}(t)\boldsymbol{\xi}(t)$ ,  $\boldsymbol{\xi}(\cdot) \in \mathbb{U}$  a.e., with time being the cost functional. The advantage of this point of view is that standard results and tools from optimal control theory can be applied immediately. For example, if  $\mathbb{U} \subseteq \mathfrak{g}$  is compact convex, then distance minimizing paths  $t \mapsto \mathbf{P}(t)$  always exist within the class of absolutely continuous functions, i.e.,  $\mathbf{P}^{-1}\dot{\mathbf{P}}$  is  $L^{\infty}$ , but not necessarily  $C^0$ . Thus shortest paths may have corners, cf. [Mie02b] for an example. Typically, corners appear when the boundary of  $\mathbb{U}$  is not strictly convex. In particular, this always happens in the case of single crystal plasticity where  $\widetilde{\Delta}$  is piecewise linear, so  $\mathbb{U}$  is a convex polyhedron. We note that  $\mathbb{U}$  need not have interior points, it suffices that  $\mathbb{U}$  generates  $\mathfrak{g}$  as a Lie algebra.

The **Pontrjagin Maximum Principle (PMP)** as a first order necessary condition for optimality is a powerful tool for finding shortest paths. For systems on Lie groups it takes a particularly simple form, cf. [Jur95,Mit95], for example. In some sense the (PMP) is the flow rule, but our point of view will give additional geometric insight.

# The (PMP) and its relation to the flow rule

Given  $\mathbb{U} \subseteq \mathfrak{g}$  we define the **optimal Hamiltonian**  $\mathcal{H} \colon \mathfrak{g}^* \to \mathbb{R}$ , as follows:

$$\mathcal{H}(\boldsymbol{\eta}) = \min_{\boldsymbol{\xi} \in \mathbb{U}} (\boldsymbol{\eta} : \boldsymbol{\xi}).$$

Let  $\widetilde{\mathbb{Q}} = \{ \eta \in \mathfrak{g}^* \mid \mathcal{H}(\eta) \geq -1 \}$ . If  $\mathbb{U}$  is convex and  $\mathbb{U} = -\mathbb{U}$ , then  $\widetilde{\mathbb{Q}}$  is simply the polar of U.

Now let I be an interval and assume that  $P: I \to \mathfrak{G}$  is a length minimizing path. Set  $\xi = \mathbf{P}^{-1}\dot{\mathbf{P}} \in L^{\infty}(I,\mathbb{U})$ . Then the (PMP) yields an absolutely continuous curve  $\eta(t) \in \mathfrak{g}^*$  with the following properties:

- (0) Nontriviality:  $\eta \neq 0$  in I,
- (1) Adjoint equation:  $Ad(\mathbf{P}^{-1}(t))^* \eta(t) \equiv \text{const} \in \mathfrak{g}^*$ ,
- (2) Minimizing condition: η(t):ξ(t) = min {η(t):ξ̃ | ξ̃ ∈ U},
  (3) Constant Hamiltonian: H(η(t)) ≡ const, either -1, or 0.

These conditions relate to the classical flow rules as follows: by (3) the curve  $\eta(t)$  evolves on a level set of  $\mathcal{H}$ , either  $\{\mathcal{H}=0\}$ , or  $\{\mathcal{H}=-1\}=\partial\mathbb{Q}$ . The latter is the **yield surface**, this becomes even more evident if one compares (3) with Eqn. (2). Although  $\mathcal{H}(\eta) \equiv 0$  is possible, this occurs only under very degenerate circumstances—it never occurs, for example, if U contains a zeroneighborhood. The **flow rule** (cf. Eqn. (4a)) is encoded in (1) and (2). The latter implies that  $\xi(t) \in \partial \mathcal{H}(\eta(t))$ . We stated the adjoint equation (1) already in integrated form using the adjoint action of  $\mathfrak{G}$  on  $\mathfrak{g}$ , resp., the induced action on  $\mathfrak{g}^*$ . For  $\mathfrak{G} = \mathrm{SL}(d)$  and  $\mathfrak{g} = \mathfrak{sl}(d)$  the adjoint action is simply conjugation:  $Ad(\mathbf{P})\xi = \mathbf{P}\boldsymbol{\xi}\mathbf{P}^{-1}$ . Identifying  $\mathfrak{sl}(d)^*$  with  $\mathfrak{sl}(d)$  via the trace form  $\eta: \boldsymbol{\xi} = \operatorname{tr}(\boldsymbol{\eta}^{\mathsf{T}} \boldsymbol{\xi})$  one may also write  $\operatorname{Ad}(\mathbf{P}^{-1})^* \boldsymbol{\eta} = \mathbf{P}^{-\mathsf{T}} \boldsymbol{\eta} \mathbf{P}^{\mathsf{T}}$ .

#### 3.2 The isotropic two-dimensional case

This case relates to isotropic plasticity of Prandtl-Reuß type using the von Mises flow rule. The plastic tensor **P** lies in  $\mathfrak{G} = \mathrm{SL}(d)$  and the material symmetry-group is  $\mathfrak{S} = O(d)$ , see (Sy4). From (Sy2) and (Sy4) one obtains that  $\Delta(\xi) = \Delta(\mathbf{R}\xi\mathbf{R}^{\mathsf{T}})$  for all  $\xi \in \mathfrak{sl}(d)$ ,  $\mathbf{R} \in \mathrm{SO}(d)$ . If one considers Riemannian metrics then  $\widetilde{\Delta}(\boldsymbol{\xi})$  can be put into the general form

$$\widetilde{\Delta}(\boldsymbol{\xi}) = (\alpha |\boldsymbol{\xi}_{\text{sym}}|^2 + \beta |\boldsymbol{\xi}_{\text{anti}}|^2)^{1/2} \text{ with } \boldsymbol{\xi}_{\text{sym}} = \frac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\xi}^{\mathsf{T}}), \ \boldsymbol{\xi}_{\text{anti}} = \frac{1}{2}(\boldsymbol{\xi} - \boldsymbol{\xi}^{\mathsf{T}}).$$
 (5)

It is shown in [Mie02b] that a curve is a shortest path if and only if it has the form

$$\mathbf{P}(t) = \mathbf{P}(0) M_{\beta/\alpha}(t\boldsymbol{\xi}) \text{ where } M_{\delta}(\boldsymbol{\xi}) = \mathrm{e}^{\boldsymbol{\xi}_{\mathrm{sym}} - \delta \boldsymbol{\xi}_{\mathrm{anti}}} \mathrm{e}^{(1+\delta)\boldsymbol{\xi}_{\mathrm{anti}}}.$$

As a consequence, the dissipation distance associated with  $\widetilde{\Delta}$  from (5) reads

$$\widetilde{D}(\mathbf{P}) = \min \{ \widetilde{\Delta}(\boldsymbol{\xi}) \mid \mathbf{P} = M_{\beta/\alpha}(\boldsymbol{\xi}) \}.$$

For symmetric, positive definite matrices  $\mathbf{P} = \mathbf{P}^{\mathsf{T}} > 0$  we find

$$\widetilde{D}(\mathbf{P}) = \sqrt{\alpha} |\log \mathbf{P}| = \sqrt{\alpha} (\log \mathbf{P} : \log \mathbf{P})^{1/2}.$$

Using the polar decomposition  $\mathbf{P} = \mathbf{R}\mathbf{U}$  with  $\mathbf{R} \in \mathrm{SO}(d)$  and  $\mathbf{U} = \mathbf{U}^\mathsf{T} > 0$  together with the triangle inequality we arrive at the explicit estimate

$$\min\{\widetilde{D}(\mathbf{R}), \widetilde{D}(\mathbf{U})\} \le \widetilde{D}(\mathbf{P}) \le \widetilde{D}(\mathbf{R}) + \widetilde{D}(\mathbf{U}),$$

where  $\widetilde{D}(\mathbf{U}) = \frac{1}{2}\sqrt{\alpha} |\log(\mathbf{U}^{\mathsf{T}}\mathbf{U})| = \frac{1}{2}\sqrt{\alpha} |\log(\mathbf{P}^{\mathsf{T}}\mathbf{P})|$ . Thus we see that for large shears  $\mathbf{P} = \mathbf{1} + \gamma \mathbf{n} \otimes \mathbf{m}$  the dissipation distance  $\widetilde{D}(\mathbf{P})$  grows at most like  $\log |\gamma|$  for  $\gamma \to \infty$ .

An important role in isotropic plasticity plays the case of zero plastic spin. This is realized by  $\alpha = 1$  and  $\beta = \infty$  in (5), or more precisely, on  $\mathfrak{sl}(d) = T_1(\mathrm{SL}(d))$  we set

$$\widetilde{\Delta}_{
m no\;spin}(oldsymbol{\xi}) = \left\{ egin{array}{ll} |oldsymbol{\xi}_{
m sym}| & {
m if}\; oldsymbol{\xi}_{
m anti} = oldsymbol{0}, \ \infty & {
m otherwise}. \end{array} 
ight.$$

The associated geodesic curves are  $\mathbf{P}(t) = \mathbf{P}(0)e^{t(\boldsymbol{\sigma}-\boldsymbol{\omega})}e^{t\boldsymbol{\omega}}$  with  $\boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathsf{T}}$  and  $\boldsymbol{\omega} = -\boldsymbol{\omega}^{\mathsf{T}}$ . Note that  $\mathbf{P}(t)^{-1}\dot{\mathbf{P}}(t) = e^{-t\boldsymbol{\omega}}\boldsymbol{\sigma}e^{t\boldsymbol{\omega}}$  is not constant but gives a constant and finite  $\Delta = \widetilde{\Delta}(\mathbf{P}(t)^{-1}\dot{\mathbf{P}}(t)) = |\boldsymbol{\sigma}|$ . In particular,  $\mathbf{P}(0)^{-1}\mathbf{P}(t)$  can reach every matrix in  $\mathrm{SL}(d)$ , not just symmetric ones. We find

$$\widetilde{D}_{\text{no spin}}(\mathbf{P}) = \min \left\{ |\boldsymbol{\sigma}| \mid \boldsymbol{\sigma} = \boldsymbol{\sigma}^{\mathsf{T}} \text{ and there exists } \boldsymbol{\omega} = -\boldsymbol{\omega}^{\mathsf{T}} \right\}.$$
(6)
such that  $\mathbf{P} = e^{\boldsymbol{\sigma} - \boldsymbol{\omega}} e^{\boldsymbol{\omega}}$ 

For d=2 the dissipation distances  $\widehat{D}_{\text{no spin}}$  can be calculated more explicitly. For  $\mathbf{P} \in \text{SL}(2)$  we have

$$\widetilde{D}_{\text{no spin}}(\mathbf{P}) = \min \left\{ \rho \geq 0 \mid \text{ there exists } \gamma \in \mathbb{R} \text{ such that } N(\rho, \gamma) = \mathbf{P} : \mathbf{P} \text{ and } T(\rho, \gamma) = \operatorname{tr} \mathbf{P} \right\}$$

where the functions N and T are defined via

$$C(t) = \begin{cases} \cosh \sqrt{t} & \text{for } t \ge 0, \\ \cos \sqrt{-t} & \text{for } t \ge 0, \end{cases} \quad \text{and} \quad S(t) = \begin{cases} \frac{\sinh \sqrt{t}}{\sqrt{t}} & \text{for } t > 0 \\ 1 & \text{for } t = 0 \\ \frac{\sin \sqrt{-t}}{\sqrt{-t}} & \text{for } t < 0 \end{cases}$$

as  $T(\rho,\gamma)=2(\cos\gamma\,C(\rho^2-\gamma^2)+\gamma\sin\gamma\,S(\rho^2-\gamma^2))$ , and  $N(\rho,\gamma)=2(1+2\rho^2[S(\rho^2-\gamma^2)]^2)$ .

It actually suffices to consider  $\gamma \in [0, \sqrt{\pi^2 + \rho^2}]$  in the minimum defining  $\widetilde{D}_{\text{no spin}}$ . For instance, for a rotation  $\mathbf{R} = \begin{pmatrix} \cos \phi & \sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix}$  with  $\phi \in [-\pi, \pi]$ , we get  $\widetilde{D}(\mathbf{R}) = \sqrt{|\phi|(2\pi + |\phi|)}$ . In particular, for  $\phi = \pi$  we have  $\widetilde{D}(-1) = \sqrt{3}\pi$  which is obtained with  $\rho = \sqrt{3}\pi$  and  $\gamma = 2\pi$  and the geodesic curve  $\mathbf{P}(t) = \mathrm{e}^{t(\sigma - \omega)}\mathrm{e}^{t\omega}$  with  $\sigma = \begin{pmatrix} \rho & 0 \\ 0 & -\rho \end{pmatrix}$  and  $\omega = \begin{pmatrix} 0 & \gamma \\ -\gamma & 0 \end{pmatrix}$ .

# 3.3 Single-crystal plasticity

In single–crystal plasticity the plastic flow occurs through plastic slip induced by movements of dislocations. Let  $\mathbf{S}^{\alpha} = \mathbf{d}^{\alpha} \otimes \mathbf{n}^{\alpha}$ ,  $\alpha = 1, ..., m$ , be the m slip systems where  $\mathbf{n}^{\alpha}$  is the unit normal to the  $\alpha$ -th slip plane and  $\mathbf{d}^{\alpha}$  is the slip direction with  $|\mathbf{d}^{\alpha}| = 1$  and  $\mathbf{d}^{\alpha} \cdot \mathbf{n}^{\alpha} = 0$ . All plastic flow has the form

$$\dot{\mathbf{P}} = \mathbf{P} \sum_{\alpha=1}^{m} \nu_{\alpha} \mathbf{S}^{\alpha}$$

where the slip rates  $\nu_{\alpha}$  are taken to be positive. This means we formally distinguish the slip systems  $\mathbf{S}^{\alpha}$  and  $-\mathbf{S}^{\alpha}$ .

The crystal symmetry group  $\mathfrak{S} \subset \mathrm{O}(d)$  is discrete and associates a permutation  $\pi_{\mathbf{R}} \in \mathrm{Perm}(m)$  to each  $\mathbf{R} \in \mathfrak{S}$  such that  $\pi_{\mathbf{R}\widehat{\mathbf{R}}} = \pi_{\mathbf{R}} \circ \pi_{\widehat{\mathbf{R}}}$  (composition of permutations) and

$$(\mathbf{R}\mathbf{d}^{\alpha},\mathbf{R}\mathbf{n}^{\alpha}) = (\mathbf{d}^{\pi_{\mathbf{R}}(\alpha)},\mathbf{n}^{\pi_{\mathbf{R}}(\alpha)}) \quad \Longleftrightarrow \quad \mathbf{S}^{\pi_{\mathbf{R}}(\alpha)} = \mathbf{R}\mathbf{S}^{\alpha}\mathbf{R}^{\mathsf{T}}.$$

The set of all slip systems  $\{ \mathbf{S}^{\alpha} \mid \alpha = 1, \dots, m \}$  determines the associated Lie algebra  $\mathfrak{g}$  (and hence the Lie group  $\mathfrak{G} \subset \mathrm{GL}_+(d)$ ) as the smallest Lie algebra containing all slip systems:

$$S := \operatorname{span} \{ \mathbf{S}_{\alpha} \mid \alpha = 1, \dots, m \} \subset \mathfrak{g} = \mathbf{T_1} \mathfrak{G}.$$

Note that  $\mathfrak{g}$  may be strictly bigger than S, as is seen in Example 1 where  $\dim S = 2 < \dim \mathfrak{g} = 3$ . From  $\mathbf{d}^{\alpha} \cdot \mathbf{n}^{\alpha} = 0$  we know  $\operatorname{tr}(\mathbf{S}^{\alpha}) = 0$  and hence  $\mathfrak{g} \subset \mathfrak{sl}(d)$  and  $\mathfrak{G} \subset \operatorname{SL}(d)$ .

We now postulate the dissipation metric and then show that it gives rise to the classical single–crystal flow rule for the resolved shear stresses  $\tau_{\alpha}$  in each slip system. With  $\boldsymbol{\xi} = \mathbf{P}^{-1}\dot{\mathbf{P}}$  the dissipation is

$$\widetilde{\Delta}(\boldsymbol{\xi}) = \min\{\sum_{\alpha=1}^{m} \kappa_{\alpha} \gamma_{\alpha} \mid \gamma_{\alpha} \geq 0, \; \boldsymbol{\xi} = \sum_{\alpha=1}^{m} \gamma_{\alpha} \mathbf{S}^{\alpha} \}$$

where  $\kappa_{\alpha} > 0$  are given threshold parameters, see [OR99,Gur00]. Since  $\widetilde{\Delta}(\mathbf{S}^{\alpha}) = \kappa_{\alpha}$ , the associated set  $\{\widetilde{\Delta} \leq 1\}$  is  $\mathbb{U} = \operatorname{conv}(\{\kappa_{\alpha}^{-1} \mathbf{S}^{\alpha} \mid \alpha = 1 \dots m\})$ . Computing the dissipation distance  $\widetilde{D}(\mathbf{P})$  can be considered as an optimal factorization problem: find  $k \in \mathbb{N}$ ,  $t_1, \dots, t_k \in \mathbb{R}^+$ , and  $\boldsymbol{\xi}_1 \dots \boldsymbol{\xi}_k \in \{\kappa_{\alpha}^{-1} \mathbf{S}^{\alpha} \mid \alpha = 1 \dots m\}$  such that  $\mathbf{P} = e^{t_1 \boldsymbol{\xi}_1} \dots e^{t_k \boldsymbol{\xi}_k}$  and  $\sum_k |t_k|$  is minimal.

The associated elastic domain  $\widehat{\mathbb{Q}}(\mathbf{P})$  is formulated in the thermodynamically conjugate variables  $\mathbf{Q} = -\partial_{\mathbf{P}}\widehat{\psi}$ . The invariant form  $\widetilde{\mathbb{Q}}$  using  $\boldsymbol{\eta} = \det \mathbf{P}^{\mathsf{T}} \mathbf{Q}$  is given by

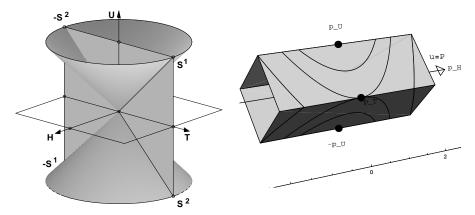
$$\widetilde{\mathbb{Q}} = \{ \boldsymbol{\eta} \in \mathfrak{sl}(d)^* \mid \kappa_{\alpha} + \mathbf{S}^{\alpha} : \boldsymbol{\eta} \leq 0 \text{ for } \alpha = 1, \dots, m \}.$$

Hence the elastic domain is characterized by one yield condition for each slip system  $\mathbf{S}^{\alpha}$ . Denoting by  $\tau_{\alpha} = \mathbf{S}^{\alpha} : \boldsymbol{\eta}$  the resolved shear stress, the slip system  $\mathbf{S}^{\alpha}$  becomes active  $(\gamma_{\alpha} > 0)$  only if  $\tau_{\alpha} = \kappa_{\alpha} > 0$ .

Example 1. [Square lattice in d = 2.] Consider d = 2 and

$$\widetilde{\varDelta}(\left(\begin{smallmatrix}\alpha & \beta \\ \gamma & -\alpha\end{smallmatrix}\right)) = \left\{ \begin{array}{cc} |\beta| + |\gamma| & \text{if } \alpha = 0, \\ \infty & \text{otherwise.} \end{array} \right.$$

This corresponds to the four slip systems  $\{\pm \mathbf{S}^1, \pm \mathbf{S}^2\}$  with  $\mathbf{S}^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ 



**Fig. 1.** The set  $\mathbb{U}$ , the yield surface  $\partial \widetilde{\mathbb{Q}}$ , and the flow rule for four 2D-slip systems

and  $\mathbf{S}^2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ . Here we have  $\mathbb{U} = \operatorname{conv}(\pm \mathbf{S}^1, \pm \mathbf{S}^2) \subseteq \mathfrak{sl}(2)$ . The Lie algebra  $\mathfrak{sl}(2)$  is a 3-dimensional vector space. For visualization purposes we use the basis  $\mathbf{H} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ,  $\mathbf{T} = \mathbf{S}^1 + \mathbf{S}^2$  and  $\mathbf{U} = \mathbf{S}^1 - \mathbf{S}^2$ . The set  $\{\boldsymbol{\xi} \in \mathfrak{sl}(2) \mid \det(\boldsymbol{\xi}) = 0, \ \boldsymbol{\xi} \neq 0\}$  of all possible slip systems is the boundary of a Lorentzian double cone. Figure 1 shows this double cone and the set  $\mathbb{U}$ . The horizontal plane  $\mathbb{R}\mathbf{H} + \mathbb{R}\mathbf{T}$  is the set of symmetric matrices (in  $\mathfrak{sl}(2)$ ) while the vertical axis is the set of skew-symmetric matrices. Using a dual basis for  $\mathfrak{sl}(2)^*$  we depicted the yield surface  $\partial \mathbb{Q}$  (which is a cylinder over a diamond square) and some integral curves of the flow rule. A careful analysis of the information provided by the (PMP) shows that for all geodesic curves  $t \mapsto \mathbf{P}(t)$  the curve  $\boldsymbol{\xi}(t) = \mathbf{P}(t)^{-1}\dot{\mathbf{P}}(t) \in \mathbb{U}$  is piecewise constant, and

$$\boldsymbol{\xi}(t) \in \left\{ \pm \mathbf{S}^1, \pm \mathbf{S}^2, \pm \frac{1}{2}(\mathbf{S}^1 + \mathbf{S}^2), \pm \frac{1}{2}(\mathbf{S}^1 - \mathbf{S}^2) \right\}.$$

Actually one obtains much more detailed information about the switching behavior of  $\xi(t)$ . We say that  $\xi(t)$  is a **bang-bang control** if it switches only between the vertices of  $\mathbb{U}$ . Otherwise, we call  $\xi(t)$  a **singular control**. From the (PMP) we obtain two types of bang-bang controls:

alternating:  $\xi(t)$  alternates between  $\mathbf{S}^1, -\mathbf{S}^2$  (or between  $-\mathbf{S}^1, \mathbf{S}^2$ ), and the time  $\tau$  between successive switches is constant,  $\tau \in (0, 2\sqrt{2})$ .

**cycling:**  $\xi(t)$  switches cyclically from vertex to vertex (of  $\mathbb{U}$ ), either clockwise or anti-clockwise. Again the time between successive switches is constant,  $\tau \in (0, \sqrt{2})$ .

There are two types of singular controls:

trivial:  $\xi(t) \equiv \pm \frac{1}{2} (\mathbf{S}^1 - \mathbf{S}^2)$  is constant;

singular:  $\xi(t)$  switches between  $\pm \mathbf{S}^1, \pm \mathbf{S}^2$ , and  $\pm \frac{1}{2}(\mathbf{S}^1 + \mathbf{S}^2)$ , but the switching patterns are more complicated although not arbitrary, see [Mit02a] for the details.

These singular controls are difficult to observe in numerical simulations. Depending on the discretization scheme it is most likely, that only the bangbang-controls are detected.

It is therefore important to emphasize that the singular controls  $\mathbf{do}$  provide geodesics. For example,  $\mathbf{P}(t) = \mathrm{e}^{\frac{t}{2}(\mathbf{S}^1 + \mathbf{S}^2)}$  is length minimizing for all t. More important, the set of  $\mathbf{P}_0 \in \mathrm{SL}(2)$  such that a length-minimizing path from  $\mathbf{1}$  to  $\mathbf{P}_0$  is either alternating or cycling, is compact and not even a neighborhood of  $\mathbf{1}$ . It also turns out that the **trivial** controls  $(\boldsymbol{\xi} \equiv \pm \frac{1}{2}(\mathbf{S}^1 - \mathbf{S}^2)$  constant) do not generate length minimizing paths. So geodesics have  $\boldsymbol{\xi}(t) \in \{\pm \mathbf{S}^1, \pm \mathbf{S}^2, \pm \frac{1}{2}(\mathbf{S}^1 + \mathbf{S}^2)\}$ .

For a fully detailed analysis of  $\widetilde{D}$  we refer to [Mit02a]. There it is shown that geodesics have at most 5 switches and which switching patterns have to be considered. We would like to emphasize that in the present example  $\widetilde{D}$  is algorithmically available, and its computation is inexpensive.

Similar results can be obtained for more general slip systems.

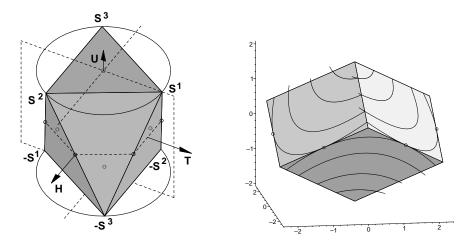


Fig. 2. The set  $\mathbb U$  and the yield surface  $\partial \mathbb Q$  for the hexagonal lattice

Example 2. [Hexagonal lattice.] Here we consider 6 slip systems along the sides of an equilateral triangle. A suitable setting is  $\mathbb{U} = \text{conv}(\pm \mathbf{S}^1, \pm \mathbf{S}^2, \pm \mathbf{S}^3)$ with  $\mathbf{S}^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ ,  $\mathbf{S}^2 = \mathbf{R}\mathbf{S}^1\mathbf{R}^\mathsf{T}$ ,  $\mathbf{S}^3 = \mathbf{R}^\mathsf{T}\mathbf{S}^1\mathbf{R}$ , where  $\mathbf{R} = \begin{pmatrix} \cos \pi/3 & \sin \pi/3 \\ -\sin \pi/3 & \cos \pi/3 \end{pmatrix}$ . The polytope U has the combinatorial structure of an octahedron, it is shown in Figure 2. There are 6 vertices, 8 (triangular) faces, and 6+8-2=12edges (Euler's formula for polyhedra). The "top" and "bottom" triangles  $\pm \operatorname{conv}(\mathbf{S}^1, \mathbf{S}^2, \mathbf{S}^3)$  are equilateral while the other triangles are isosceles. The polar  $\widetilde{\mathbb{Q}}$  is the dual polytope of  $\mathbb{U}$ . Therefore its combinatorial structure is that of a cube with 8 vertices, 6 (quadrilateral) faces, and 8+6-2=12edges, cf. Figure 2 which also shows some integral curves of the flow rule. The overshooting tips indicate the flow direction and which switches occur. As in the previous example one obtains from the (PMP) that  $\xi(t) = \mathbf{P}(t)^{-1}\mathbf{P}(t)$  is piecewise constant for length-minimizing  $\mathbf{P}(t)$ . Apart from the 6 possibilities we get from the vertices of U there are an additional 6 possibilities (each corresponding to a vertex of  $\widetilde{\mathbb{Q}}$ , resp., a face of  $\mathbb{U}$ ) plus 6 possibilities corresponding to (some) edges of  $\mathbb{U}$ , resp.  $\widetilde{\mathbb{O}}$ . Thus we have a total of 18 possible values for  $\xi$ . Generically,  $\xi(t)$  cycles through the vertices of a single face of  $\mathbb{U}$ in a certain order. For example, on the "top" face  $conv(S^1, S^2, S^3)$  the switching sequence is  $S^1 \rightsquigarrow S^3 \rightsquigarrow S^2 \cdots$ ; on the "lateral" face  $conv(S^1, -S^2, -S^3)$ the switching sequence is  $S^1 \rightsquigarrow -S^2 \rightsquigarrow -S^3 \dots$  There are trivial cases (i.e.  $\xi$ constant) corresponding to the vertices of Q. Nevertheless, it turns out that none of these is optimal. Finally, we also get more complicated singular cases. We will provide the details in the forthcoming paper [Mit02b]. Although computation of D is technically more difficult than for the square lattice, all the obstacles can be overcome.

Considering the previous two examples it is natural to ask whether it is true in general that for arbitrary 2D-slips systems the length minimizing paths have piecewise constant  $\boldsymbol{\xi} = \mathbf{P}^{-1}\dot{\mathbf{P}}$ . This is actually true, but it is by no means obvious because it is definitely  ${\bf not}$  true for arbitrary polyhedra  $\mathbb{U}\subseteq$ st(2). For example, let  $\boldsymbol{\xi}_1 = \begin{pmatrix} 1 & 0 \\ 2 & -1 \end{pmatrix}$ ,  $\boldsymbol{\xi}_2 = \begin{pmatrix} 1 & 0 \\ -2 & -1 \end{pmatrix}$ ,  $\boldsymbol{\xi}_3 = -\boldsymbol{\xi}_1^\mathsf{T}$ ,  $\boldsymbol{\xi}_4 = -\boldsymbol{\xi}_2^\mathsf{T}$ , and  $\mathbb{U} = \mathrm{conv}(\boldsymbol{\xi}_1, \dots, \boldsymbol{\xi}_4)$ . Since  $\mathrm{tr}(\boldsymbol{\xi}_j^\mathsf{T} \boldsymbol{\xi}_k) = -2$  for  $j \neq k$ , we can write  $\mathbb{Q} = \operatorname{conv}(\eta_1, \dots, \eta_4)$  with  $\eta_j = \frac{1}{2} \xi_j$ . Here it may happen, for instance, that  $\xi(t) \in \text{conv}(\xi_1, \xi_2)$  varies arbitrarily. The geometric reason for this is that  $\mathbb{R}\boldsymbol{\xi}_1 + \mathbb{R}\boldsymbol{\xi}_2 \subseteq \mathfrak{sl}(2)$  is a 2-dimensional subalgebra. Speaking in geometric terms, degeneracies occur if one of the edges of the polytope U lies in a 2-dimensional subalgebra of  $\mathfrak{sl}(2)$ . It is well-known that the 2-dimensional subalgebras in  $\mathfrak{sl}(2)$  are precisely the tangent planes of the double cone (depicted in Fig. 1). Thus for slip systems these degeneracies never occur because for two elements  $S^1, S^2$  of the double cone the segment  $conv(S^1, S^2)$  is tangential to the cone iff  $S^1$  and  $S^2$  are collinear. Moreover, for general slip systems the combinatorial structure of the polytope  $\mathbb{U} = \text{conv}(\mathbf{S}^1, \dots, \mathbf{S}^m)$  gives an apriori bound for the number of possible values of  $\boldsymbol{\xi}$ . If, say,  $\mathbb{U}$  has  $f_0$  vertices,  $f_1$  edges and  $f_2$  faces, then the number of possible values of  $\xi$  is bounded by  $f_0 + f_1 + f_2$ .

We get at most one singular control for each edge of  $\mathbb{Q}$  (i.e., each face of  $\mathbb{U}$ ) and each edge of  $\mathbb{Q}$ , resp.  $\mathbb{U}$ . As  $f_0 - f_1 + f_2 = 2$  (Euler's polyhedra formula)  $f_0 + f_1 + f_2 = 2(f_0 + f_2 - 1)$ .

# 4 Isotropic hardening

Finally we want to address the question of hardening. In general this is a difficult question since many hardening variables may be needed, in particular in the case of latent hardening [OR99,ORS00]. On the other hand, systems without any hardening are too soft to withstand any nontrivial stresses, since the reduced functionals (cf. [OR99,CHM02,Mie02a]) grow only logarithmic at infinity.

Here we propose a simple model of isotropic hardening using a scalar variable only. In the case of isotropic material this reduces to the classical isotropic Prandtl–Reuß–von Mises model. Thus, we consider the internal variables  $(\mathbf{P},p) \in \mathfrak{G} \times [0,\infty)$  with an infinitesimal dissipation potential  $\widehat{\Delta}$  of the form

$$\widehat{\Delta}((\mathbf{P},p),(\dot{\mathbf{P}},\dot{p})) = \left\{ \begin{array}{ll} \widetilde{\Delta}(\mathbf{P}^{-1}\dot{\mathbf{P}}) \text{ if } \widetilde{\Delta}(\mathbf{P}^{-1}\dot{\mathbf{P}}) \leq a(p)\dot{p}, \\ \infty & \text{otherwise}, \end{array} \right.$$

where  $a:[0,\infty[\to]0,\infty[$  is assumed to be continuous. Here  $\widetilde{\Delta}:\mathfrak{g}\to[0,\infty]$  is convex and homogeneous of degree 1. By  $\widetilde{D}:\mathfrak{G}\to[0,\infty]$  we denote the global dissipation distance associated with  $\widetilde{\Delta}$ . Moreover, by  $\widetilde{\Delta}^*:\mathfrak{g}^*\to[0,\infty]$  we denote its polar function, i.e.,  $\widetilde{\Delta}^*(\eta):=\max\{\boldsymbol{\xi}:\eta\mid\widetilde{\Delta}(\boldsymbol{\xi})\leq 1\}$ .

The left-invariant elastic domain  $\widehat{\mathbb{Q}}(p)$  is given by

$$\widetilde{\mathbb{Q}}(p) = \{ (\boldsymbol{\eta}, q) \in \mathfrak{g} \times \mathbb{R} \mid q < 0, \ \Delta^*(\boldsymbol{\eta}) + q < 1 + a(p) \}.$$

We see that hardening is obtained if a(p) is increasing in p. Denoting by A the primitive function of a (i.e.,  $A(p) = \int_0^p a(s) \, ds$ ) we obtain the following formula for the global dissipation distance:

$$\widehat{D}((\mathbf{P}_0, p_0), (\mathbf{P}_1, p_1)) = \begin{cases} \widetilde{D}(\mathbf{P}_0^{-1} \mathbf{P}_1) + A(p_1) - A(p_0) & \text{if } p_1 \leq p_0 + \widetilde{D}(\mathbf{P}_0^{-1} \mathbf{P}_1), \\ \infty & \text{otherwise.} \end{cases}$$

We refer to [Mie02a] for more general cases.

### References

[CHM02] C. Carstensen, K. Hackl, and A. Mielke. Nonconvex potentials and microstructure in finite-strain plasticity. *Proc. Royal Soc. London Ser. A*, 458(2018), 299-317, 2002.

[Gur00] M. E. Gurtin. On the plasticity of single crystals: free energy, microforces, plastic-strain gradients. J. Mech. Phys. Solids, 48(5), 989-1036, 2000.

- [HH02] K. HACKL and U. HOPPE. On the calculation of microstructures for inelastic materials using relaxed energies. *Proc. of IUTAM Symposium on Computational Mechanics of Solid Materials at Large Strains (Aug. 2001)*, to appear.
- [Jur95] V. Jurdjevic. Non-euclidean elastica. Am. J. Math, 117, 93–124, 1995.
- [ML01] C. MIEHE AND M. LAMBRECHT. Analysis of Microstructure development in shearbands by energy relaxation of incremental stress potentials: large-strain theory for generalized standard solids. Report No. 01-I-10, Inst. Mech., Univ. Stuttgart., 2001.
- [MSL01] C. MIEHE, J. SCHOTTE, AND M. LAMBRECHT. Homogenization of inelastic solid materials at finite strains based on incremental minimization principles. Application to the texture analysis of polycrystals. Report No. 01-I-07, Inst. Mech., Univ. Stuttgart., 2001.
- [Mie02a] A. MIELKE. Energetic formulation of multiplicative elastoplasticity using dissipation distances. J. Mech. Physics Solids, 2002. Submitted.
- [Mie02b] A. MIELKE. Finite elastoplasticity, Lie groups and geodesics on SL(d). In P. Newton, A. Weinstein, and P. Holmes, editors, Geometry, Dynamics, and Mechanics. Springer-Verlag, 2002. In press.
- [Mit95] D. MITTENHUBER. Applications of the Maximum Principle to problems in Lie semigroups. In K.H. Hofmann, J.D. Lawson, and E.B. Vinberg, editors, Semigroups in Algebra, Geometry and Analysis. de Gruyter, 1995.
- [Mit02a] D. MITTENHUBER. The dissipation distance for a 2D single crystal with two symmetric slip systems. In preparation, 2002.
- [Mit02b] D. MITTENHUBER. Dissipation distances for 2D single crystals: The hexagonal lattice. In preparation, 2002.
- [OR99] M. ORTIZ and E. REPETTO. Nonconvex energy minimization and dislocation structures in ductile single crystals. J. Mech. Phys. Solids, 47(2), 397–462, 1999.
- [ORS00] M. ORTIZ, E. REPETTO, and L. STAINIER. A theory of subgrain dislocation structures. J. Mech. Physics Solids, 48, 2077–2114, 2000.
- [PBGM62] L.S. PONTRJAGIN, V.G. BOLTYANSKI, R.V. GAMKRELIDZE, and E.F. MISHCHENKO. The Mathematical Theory of Optimal Processes. Wiley Interscience, 1962.