Rend. Sem. Mat. Univ. Pol. Torino
Vol. 58, 1 (2000)
Geom., Cont. and Micros., I

E. Binz - D. Socolescu

MEDIA WITH MICROSTRUCTURES AND THERMODYNAMICS FROM A MATHEMATICAL POINT OF VIEW

Abstract. Based on the notion of continua with microstructures we introduce the notion of microstructures on discrete bodies. Using the analogy with of differential forms on discrete media we develop the discrete virtual work and the thermodynamics in the sense of Caratheodory.

1. Continua with microstructures

Let B be a medium, i.e. a three dimensional compact, differentiable manifold with boundary. In the case of classical continuum mechanics this medium is thought to be moving and deforming in $\mathbb{R}^3$. A configuration is then a smooth embedding $\Phi : B \to \mathbb{R}^3$. The configuration space is then either $\mathcal{E}(B, \mathbb{R}^3)$, the collection of all smooth embeddings from B into $\mathbb{R}^3$, a Fréchet manifold, or, for physical reasons, a subset of $\mathcal{E}(B, \mathbb{R}^3)$ which we denote by $conf\ (B, \mathbb{R}^3)$. This classical setting can be generalized to media with microstructures.

A medium B with microstructure is thought as a medium whose points have internal degrees of freedom. Such a medium was recently modelled by a specified principal bundle $P \stackrel{\pi}{\to} B$ with structure group H, a compact Lie group ([3])

Accordingly the medium B with microstructure is thought to be moving and deforming in the ambient space $\mathbb{R}^3$ with microstructure, which is modelled by another specified principal bundle $Q \stackrel{\omega}{\to} \mathbb{R}^3$, with structure group G, a Lie group containing H. A configuration is then a smooth, H-equivariant, fibre preserving embedding $\tilde{\Phi} : P \to Q$, i.e.

$$\tilde{\Phi}(p, h) = \tilde{\Phi}(p) \cdot h, \qquad \forall\ p \in P,\ \ \forall\ h \in H.$$

The configuration space is then either $\mathcal{E}(P, Q)$, i.e. the collection of all these configurations, or again for physical reasons $Conf(P, Q)$, a subset of $\mathcal{E}(P, Q)$. Clearly any $\tilde{\Phi} \in \mathcal{E}(P, Q)$ determines some $\Phi \in \mathcal{E}(B, \mathbb{R}^3)$ by

$$\Phi\,(\pi(p)) = \omega\left(\tilde{\Phi}(p)\right),\ \forall\ p \in P.$$

The map $\pi_{\mathcal{E}} : \mathcal{E}(P, Q) \to \mathcal{E}(B, \mathbb{R}^3)$ given by

$$\pi_{\mathcal{E}}(\tilde{\Phi})(\pi(p)) = \omega(\tilde{\Phi}(p)),\ \forall\ p \in P,\ \forall\ \tilde{\Phi} \in \mathcal{E}(P, Q),$$

is not surjective in general. For the sake of simplicity we assume in the following that $\pi_{\mathcal{E}}$ is surjective. Given two configurations $\tilde{\Phi}_1, \tilde{\Phi}_2$ in $\pi_{\mathcal{E}}^{-1}(\Phi) \subset \mathcal{E}(P, Q)$ for $\Phi \in \mathcal{E}(B, \mathbb{R}^3)$, there exists a smooth map $\tilde{g} : P \to G$, called gauge transformation, such that

$$\tilde{\Phi}_1(p) = \tilde{\Phi}_2(p) \cdot \tilde{g}(p),\ \forall\ p \in P.$$

Moreover, $\tilde{g}$ satisfies

$$\tilde{g}(p \cdot h) = h^{-1} \cdot \tilde{g}(p) \cdot h, \ \forall \ p \in P, \ \forall \ h \in H.$$

The collection G_P^H of all gauge transformations $\tilde{g}$ form a group, the so-called gauge group.

The gauge group G_P^H is a smooth Fréchet manifold. In fact $\mathcal{E}(P, Q)$ is a principal bundle over $\mathcal{E}(B, \mathbb{R}^3)$ with G_P^H as structure group.

2. Discrete systems with microstructures

In the following we show how the notion of media with microstructure dealed with above in the continuum case can be introduced in the discrete case. To this end we replace the body manifold, i.e. the medium B, by a connected, two-dimensional polyhedron $\mathbb{P}$. We denote the collection of all vertices q of $\mathbb{P}$ by $S^0\mathbb{P}$, the collection of all bounded edges e of $\mathbb{P}$ by $S^1\mathbb{P}$, and the collection of all bounded faces f of $\mathbb{P}$ by $S^2\mathbb{P}$. We assume that:

i) every edge $e \in S^1\mathbb{P}$ is directed, having e^- as initial and e^+ as final vertex, and therefore oriented,

ii) every face $f \in S^2\mathbb{P}$ is plane starshaped with respect to a given barycenter B_f and oriented. Morever, f is regarded as the plane cone over its boundary ∂f, formed with respect to B_f. This cone inherits from $\mathbb{R}^2$ a smooth linear parametrization along each ray joining B_f with the vertices of f and with distinguished points of the edges belonging to ∂f and joining these vertices, as well as a picewise smooth, linear parametrization along the boundary ∂f of f, i.e. along the edges.

A configuration of $\mathbb{P}$ is a map $\Phi : \mathbb{P} \to \mathbb{R}^3$ with the following defining properties:

i) $j : S^0\mathbb{P} \to \mathbb{R}^3$ is an embedding;

ii) if any two vertices q_1 and q_2 in $S^0\mathbb{P}$ are joined by some edge e in $S^1\mathbb{P}$, then the image $\Phi(e)$ is the edge joining $\Phi(q_1)$ and $\Phi(q_2)$;

iii) the image $\Phi(f)$ of every face f in $S^2\mathbb{P}$, regarded as the plane cone over its boundary ∂f formed with respect to B_f, is a cone in $\mathbb{R}^3$ over the corresponding boundary $\Phi(\partial f)$ formed with respect to $\Phi(B_f)$;

iv) Φ preserves the orientation of every face $f \in S^2\mathbb{P}$ and of every edge $e \in S^1\mathbb{P}$.

We denote by $\mathcal{E}(\mathbb{P}, \mathbb{R}^3)$ the collection of all configurations Φ of $\mathbb{P}$, and by $conf\left(\mathbb{P},\mathbb{R}^3\right)$ the configuration space, which is either $\mathcal{E}(\mathbb{P}, \mathbb{R}^3)$ or eventually a subset of it.

As in the continuum case we model the plyhedron $\mathbb{P}$ with microstructure by a principal bundle $P \xrightarrow{\pi} \mathbb{P}$ with structure group H, a compact Lie group, while the ambient space $\mathbb{R}^3$ with microstructure is modelled by another principal bundle $Q \xrightarrow{\omega} \mathbb{R}^3$ with structure group G, a Lie group containing H.

We note that we implement the interaction of internal variables by fixing a connection on $P \xrightarrow{\pi} \mathbb{P}$, and this can be done by using an argument similar to that one in [4]. Clearly not every closed, piecewise linear curve in $\mathbb{P}$ can be lifted to a closed, piecewise linear curve in P.

The configuration space $Conf(P, Q)$ is a subset of the collection $\mathcal{E}(P, Q)$ of smooth, H-equivariant, fibre preserving embeddings $\tilde{\Phi} : P \to Q$.

Again $Conf(P, Q)$ is a principal bundle over $conf(\mathbb{P}, \mathbb{R}^3)$ or over some open subset of it with G_P^H as structure group.

3. The interaction form and its virtual work

Let us denote by $F(S^0\mathbb{P}, \mathbb{R}^3)$ the collection of all $\mathbb{R}^3$-valued functions on $S^0\mathbb{P}$, by $A(S^1\mathbb{P}, \mathbb{R}^3)$ the collection of all $\mathbb{R}^3$-valued one-forms on $\mathbb{P}$, i.e. of all maps $\gamma : S^1\mathbb{P} \to \mathbb{R}^3$, and by $A^2\left(S^2\mathbb{P}, \mathbb{R}^3\right)$ the collection of all $\mathbb{R}^3$-valued two-forms on $\mathbb{P}$, i.e. of all maps $\omega : S^2\mathbb{P} \to \mathbb{R}^3$. We note that $F(S^0\mathbb{P}, \mathbb{R}^3)$, $A^1 S^1\mathbb{P}, \mathbb{R}^3)$ and $A^2(S^2\mathbb{P}, \mathbb{R}^3)$ are finite dimensional $\mathbb{R}$-vector spaces due to the fact that $\mathbb{P}$ has finitely many vertices, edges and faces. In all these vector spaces we can present natural bases. Indeed, given any $z \in \mathbb{R}^3$ and a fixed vertex $q \in S^0\mathbb{P}$, we define $h_q^z \in F(S^0\mathbb{P}, \mathbb{R}^3)$ as follows:

$$h_q^z(q') = \begin{cases} z \ , & \text{if } q = q' \\ 0 \ , & \text{otherwise} \ . \end{cases}$$

On the other hand, for a fixed edge $e \in S^1\mathbb{P}$ respectively a fixed face $f \in S^2\mathbb{P}$, $\gamma_e^z \in A^1(S^1\mathbb{P}, \mathbb{R}^3)$ and $\omega_f^z \in A^2(S^2\mathbb{P}, \mathbb{R}^3)$ are given in the following way:

$$\gamma_e^z(e') = \begin{cases} z \ , & \text{if } e = e' \ , \\ 0 \ , & \text{otherwise} \ , \end{cases} \qquad \omega_f^z(f') = \begin{cases} z \ , & \text{if } f = f' \ , \\ 0 \ , & \text{otherwise} \ . \end{cases}$$

If now $\{z_1, z_2, z_3\}$ is a base in $\mathbb{R}^3$, then

$$\{h_q^{z_i} \mid q \in S^0\mathbb{P}, i = 1, 2, 3\} \subset F(S^0\mathbb{P}, \mathbb{R}^3)$$

$$\{\gamma_e^{z_i} \mid e \in S^1\mathbb{P}, i = 1, 2, 3\} \subset A^1(S^1\mathbb{P}, \mathbb{R}^3)$$

and

$$\{\omega_q^{z_i} \mid f \in S^2\mathbb{P}, i = 1, 2, 3\} \subset A^2(S^2\mathbb{P}, \mathbb{R}^3)$$

are the natural bases mentioned above.

Given now a scalar product $\langle \cdot, \cdot \rangle$ on $\mathbb{R}^3$, we define the scalar product G^0, G^1 and G^2 on $F(S^0\mathbb{P}, \mathbb{R}^3)$, $A^1(S^1\mathbb{P}, \mathbb{R}^3)$ and respectively $A^2(S^2\mathbb{P}, \mathbb{R}^3)$ by

$$G^0(h_1, h_2) := \sum_{q \in S^0 P} \langle h_1(q), h_2(q) \rangle \ , \ \forall \, h_1, h_2 \in F(S^0\mathbb{P}, \mathbb{R}^3) \ ,$$

$$G^1(\gamma_1, \gamma_2) := \sum_{e \in S^1 P} \langle \gamma_1(e), \gamma_2(e) \rangle \ , \ \forall \, \gamma_1, \gamma_2 \in A^1(S^1\mathbb{P}, \mathbb{R}^3) \ ,$$

and

$$G^2(\omega_1, \omega_2) := \sum_{f \in S^2 P} \langle \omega_1(f), \omega_2(f) \rangle \ , \ \forall \, \omega_1, \omega_2 \in A^2(S^2\mathbb{P}, \mathbb{R}^3).$$

The differential dh of any $h \in F(S^0\mathbb{P}, \mathbb{R}^3)$ is a one-form on $\mathbb{P}$ given by

$$dh(e) = h(e^+) - h(e^-) \ , \ \forall \, e \in S^1\mathbb{P} \ ,$$

where e^- and e^+ are the initial and the final vertex of e.

The exterior differential $d : A^1(S^1\mathbb{P}, \mathbb{R}^3) \to A^2(S^2\mathbb{P}, \mathbb{R}^3)$ applied to any $\gamma \in A^1(S^1\mathbb{P}, \mathbb{R}^3)$ is given by

$$d\gamma(f) := \sum_{e \in \partial f} \gamma\,(e) \ \ , \ \forall \, f \in S^2\mathbb{P} \ .$$

The exterior differential $d\omega$ for any two-form ω on $\mathbb{P}$ vanishes. Associated with d and the above scalar products are the divergence operators

$$\delta : A^2(S^2\mathbb{P}, \mathbb{R}^3) \to A^1(S^1\mathbb{P}, \mathbb{R}^3)$$

and

$$\delta : A^1(S^1\mathbb{P}, \mathbb{R}^3) \to F(S^0\mathbb{P}, \mathbb{R}^3) ,$$

respectively defined by the following equations

$$G^1(\delta\omega, \alpha) = G^2(\omega, d\alpha) \quad , \quad \forall\, \omega \in A^2(S^2\mathbb{P}, \mathbb{R}^3) \text{ and } \forall\, \alpha \in A^1(S^1\mathbb{P}, \mathbb{R}^3) ,$$

and

$$G^0(\delta\alpha, h) = G^1(\alpha, dh) \quad , \quad \forall\, \alpha \in A^1(S^1\mathbb{P}, \mathbb{R}^3) \text{ and } \forall\, h \in F(S^0\mathbb{P}, \mathbb{R}^3) .$$

$d \circ d = 0$ implies $\delta \circ \delta = 0$. Elements of the form dh in $A^1(S^1\mathbb{P}, \mathbb{R}^3)$ for any $h \in F(S^0\mathbb{P}, \mathbb{R}^3)$ are called exact, while elements of the form $\delta\omega$ in $A^1(S^1\mathbb{P}, \mathbb{R}^3)$ for any $\omega \in A^2(S^2\mathbb{P}, \mathbb{R}^3)$ are called coexact.
The Laplacians Δ_0, Δ_1 and Δ_2 on $F(S^0\mathbb{P}, \mathbb{R}^3)$, $A^1(S^1\mathbb{P}, \mathbb{R}^3)$ and $A^2(S^2\mathbb{P}, \mathbb{R}^3)$ are respectively defined by

$$\Delta_i := \delta \circ d + d \circ \delta \ , \ i = 0, 1, 2 \ .$$

Due to dim $\mathbb{P} = 2$ these Laplacians, selfadjoint with respect to G^i, $i = 0, 1, 2$, simplify to $\Delta_0 = \delta \circ d$ on functions, $\Delta_1 = \delta \circ d + d \circ \delta$ on one-forms and $\Delta_2 = d \circ \delta$ on two-forms. Hence there are the following G^0, G^1- and respectively G^2-orthogonal splittings, the so called Hodge splittings [1]:

$$\begin{aligned}
A^0(S^0\mathbb{P}, \mathbb{R}^3) &= \delta A^1(S^1\mathbb{P}, \mathbb{R}^3) \oplus Harm^0(S^0\mathbb{P}, \mathbb{R}^3) , \\
A^1(S^1\mathbb{P}, \mathbb{R}^3) &= dF(S^0\mathbb{P}, \mathbb{R}^3) \oplus \delta A^2(S^2\mathbb{P}, \mathbb{R}^3) \oplus Harm^1(S^1\mathbb{P}, \mathbb{R}^3) , \\
A^2(S^2\mathbb{P}, \mathbb{R}^3) &= dA^1(S^1\mathbb{P}, \mathbb{R}^3) \oplus Harm^2(S^2\mathbb{P}, \mathbb{R}^3) .
\end{aligned}$$

Here $Harm^i(S^i\mathbb{P}, \mathbb{R}^3) := Ker\ d \cap Ker\ \delta$, $i = 0, 1, 2$. Reformulated, this says that $\beta \in Harm^i(S^i\mathbb{P}, \mathbb{R}^3)$ if $\Delta_i\beta = 0$, $i = 0, 1, 2$; we note that $\beta \in Harm^0(S^0\mathbb{P}, \mathbb{R}^3)$ is a constant function.

Letting $H^i(\mathbb{P}, \mathbb{R}^3)$ be the i-th cohomology group of $\mathbb{P}$ with coefficients in $\mathbb{R}^3$, we hence have:

$$H^i(\mathbb{P}, \mathbb{R}^3) \cong Harm^i(S^i\mathbb{P}, \mathbb{R}^3) \ , \ i = 1, 2 \ .$$

Next we introduce the stress or interaction forms, which are constitutive ingredients of the polyhedron $\mathbb{P}$. To this end we consider the interaction forces, i.e. vectors in $\mathbb{R}^3$,which act up on any vertex q, along any edge e and any face f of $\mathbb{P}$.

The collection of all these forces acting up on the vertices defines a configuration dependent function $\alpha^0(\Phi) \in F(S^0\mathbb{P}, \mathbb{R}^3)$, where $\Phi \in conf\left(\mathbb{P}, \mathbb{R}^3\right)$. Analogously the collection of all the interaction forces acting up along the edges or along the faces defines a one form $\alpha^1(\Phi) \in A^1(S^1\mathbb{P}, \mathbb{R}^3)$ or a two-form $\alpha^2(\Phi) \in A^2(S^2\mathbb{P}, \mathbb{R}^3)$ respectively. The virtual work $\mathcal{A}^i(\Phi)$ caused respectively by any distortion $\gamma^i \in A^i(S^i\mathbb{P}, \mathbb{R}^3)$, $i = 0, 1, 2$, is given by

$$\mathcal{A}^i(\Phi)(\gamma^i) = \mathcal{G}^i(\alpha^i(\Phi), \gamma^i), \ i = 0, 1, 2 \ .$$

However, it is important to point out that the total virtual work $\mathcal{A}(\Phi)$ caused by a deformation of the polyhedron $\mathbb{P}$ is given only by $\mathcal{A}^1(\Phi)(\gamma^1)+\mathcal{A}^2(\Phi)\left(\rho^2\right)$, where ρ^2 is the harmonic part of $\gamma^2 \in A^2(S^2\mathbb{P},\mathbb{R}^3)$. In order to justify it we give the virtual works $\mathcal{A}^i(\Phi)(\gamma^i),\ i=1,2,$ in accordance with the Hodge splitting for $\alpha^i(\Phi)$ and $\gamma^i,\ i=0,1,2,$ and with the definition of the divergence operators δ, the equivalent forms

$$\begin{array}{rcl}
\mathcal{G}^0(\alpha^0(\Phi),\delta\gamma^1) & = & \mathcal{G}^1(d\alpha^0(\Phi),\gamma^1),\\
\mathcal{G}^1(\alpha^1(\Phi),\gamma^1) & = & \mathcal{G}^1(d\beta^0+\delta\omega^2+\varkappa^1,\gamma^1)\\
& = & \mathcal{G}^0(\beta^0,\delta\gamma^1)+\mathcal{G}^2(\omega^2,d\gamma^1)+\mathcal{G}^1(\varkappa^1,\rho^1)\\
\mathcal{G}^2(\alpha^0(\Phi),\delta\gamma^1) & = & \mathcal{G}^2(d\beta^1+\varkappa^2,\gamma^2)=\mathcal{G}^1(\beta^1,\delta\gamma^2)+\mathcal{G}^2(\varkappa^2,\rho^2),
\end{array}$$

Here the two terms

$$\mathcal{G}^1(\varkappa^1,\gamma^1)=\mathcal{G}^1(\varkappa^1,dh^0+dh^2+\rho^1)=\mathcal{G}^1(\varkappa^1,\rho^1),$$

and

$$\mathcal{G}^2(\varkappa^2,\gamma^2)=\mathcal{G}^2(\varkappa^2,dh^1+\rho^2)=\mathcal{G}^2(\varkappa^2,\rho^2)$$

depend only on the topology of the polyhedron $\mathbb{P}$.

Comparing now the different expressions for the virtual works we get

$$\begin{array}{rcl}
\mathcal{A}^1(\Phi)\left(\gamma^1\right)+\mathcal{G}^2(\varkappa^2,\rho^2) & = & \mathcal{G}^0(\alpha^0(\Phi),\delta\gamma^1)+\mathcal{G}^2(\alpha^2(\Phi),d\gamma^1)+\\
& + & \mathcal{G}^1(\varkappa^1,\rho^1)+\mathcal{G}^2(\varkappa^2,\rho^2),
\end{array}$$

$$\begin{array}{rcl}
\alpha^0(\Phi) & = & \delta\alpha^1(\Phi),\\
\alpha^1(\Phi) & = & d\alpha^0(\Phi)+\delta\alpha^2(\Phi)+\rho^1,\\
\alpha^2(\Phi) & = & d\alpha^1(\Phi)+\rho^2.
\end{array}$$

Moreover

$$\begin{array}{rcl}
\Delta_0\alpha^0(\Phi) & = & \alpha^0(\Phi)\ ,\\
\Delta_2\alpha^2(\Phi)+\varkappa^2 & = & \alpha^2(\Phi)\ .
\end{array}$$

Accordingly, the total virtual work on $\mathbb{P}$ associated, as discussed above, with α^0, α^1 and α^2 is given by

$$\begin{array}{rcl}
\mathcal{A}(\Phi)(\gamma^1,\gamma^2) & := & \mathcal{A}^1(\Phi)(\gamma^1)+\mathcal{A}^2(\Phi)(\rho^2)\\
& = & \mathcal{G}^1(\alpha^1(\Phi),\Delta_1\gamma^1)+\mathcal{G}^1(\varkappa^1,\rho^1)+\mathcal{G}^2(\varkappa^2,\rho^2)
\end{array}$$

However, due to translational invariance

$$\alpha^i(\Phi)=\alpha^i(d\Phi),\ i=0,1,2\ .$$

For this reason we let $d\Phi$ vary in a smooth, compact and bounded manifold $K\subset dconf(\mathbb{P},\mathbb{R}^3)$ with non-empty interior. The virtual work on $\mathbb{P}$ has then the form

$$\mathcal{A}(\Phi)(\gamma^1,\gamma^2)=\mathcal{A}(d\Phi)(\gamma^1,\gamma^2)$$

for any $d\Phi\in K$ and any $\gamma^i\in A^i(S^i\mathbb{P},\mathbb{R}^3)$. Since $dconf\left(\mathbb{P},\mathbb{R}^3\right)\subset A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$ according to the Hodge splitting is not open, not all elements in $A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$ are tangent to

$dconf\left(\mathbb{P},\mathbb{R}^3\right)$. Therefore, $\mathcal{A}$ is not a one-form on $\mathcal{K}\subset dconf\left(\mathbb{P},\mathbb{R}^3\right)$, in general. To use the formalism of differential forms, we need to extend the virtual work $\mathcal{A}$ to some compact bounded submanifold $\mathcal{K}^1\subset A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$ with $\mathcal{K}\subset\mathcal{K}^1$- See [2] for details -

The one-form $\mathcal{A}(d\Phi)$ needs not to be exact, in general. We decompose accordingly $\mathcal{A}$ into

$$\mathcal{A}(d\Phi) = \ dI\,F + \Psi.$$

This decomposition is the so called Neumann one, given by

$$div\mathcal{A} = \Delta F,\ \ \mathcal{A}(\xi)\,(\nu(\xi)) = \mathbb{D}(\xi)(\nu(\xi))$$

for all ξ in the boundary $\partial\mathcal{K}^1$ of $\mathcal{K}^1$. $\mathbb{D}$ is the Fréchet derivative on $A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$, while ν is the outward directed unit normal field on ∂K^1. The differential opeators div and Δ are the divergence and respectively the Laplacian on $A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$.

4. Thermodynamical setting

This Neumann decomposition, combined with the idea of integrating factor of the heat, as presented in [1], [6] and [7], yields a thermodynamical setting.

In order to do this let us remember first that $A^1\left(S^1\mathbb{P},\mathbb{R}^3\right)$ has according to the Hodge splitting the decomposition

$$A^1\left(S^1\mathbb{P},\mathbb{R}^3\right) = dF\left(S^0\mathbb{P},\mathbb{R}^3\right)\oplus\delta A^2\left(S^2\mathbb{P},\mathbb{R}^3\right)\oplus Harm^1\left(S^1\mathbb{P},\mathbb{R}^3\right).$$

This fact implies the necessity of one additional coordinate function for the construction of the therodynamical setting. Accordingly we extend $\mathcal{K}^1$ to $\mathcal{K}_{\mathbb{R}} := \mathcal{K}^1\times\mathbb{R}$ and pull $\mathcal{A}$ back to $\mathcal{K}_{\mathbb{R}}$. The pull back is again denoted by $\mathcal{A}$.

We follow now the argument in [2] and denote by U the additional coordinate function on $\mathcal{K}_{\mathbb{R}}$: we set for the heat

$$H := \ dIU - \mathcal{A}$$

where by dI we denote here the differential on $\mathcal{K}_{\mathbb{R}}$.

Let now $\frac{1}{T}$ be an integrating factor of H; i.e.

$$H = T\ dIS \quad \text{on} \quad \mathcal{K}_{\mathbb{R}},$$

where $S:\mathcal{K}_{\mathbb{R}}\to\mathbb{R}$ is a smooth function ([2]). Next we introduce the free energy $F_{\mathcal{K}_{\mathbb{R}}}$ by setting

$$F_{\mathcal{K}_{\mathbb{R}}} := U - T\cdot S\ ,$$

yielding

$$\mathcal{A} = \ dI\,F_{\mathcal{K}_{\mathbb{R}}} - S\ dIT\ .$$

Both $F_{\mathcal{K}_{\mathbb{R}}}$ and T depend on the tuple $(\xi,U)\in\mathcal{K}_{\mathbb{R}}$. The one-form $\mathcal{A}$ on $\mathcal{K}_{\mathbb{R}}$ depends trivially on U. We think of some dependence of U on ξ, i.e. we think of a map $s:\mathcal{K}^1\to\mathbb{R}$ and restrict the above decomposition of $\mathcal{A}$ to the graph of s. s is determined by the equation

$$F_{\mathcal{K}_{\mathbb{R}}}\,(\xi,s(\xi)) = F(\xi) + F^0,$$

$\forall \xi$ in some submanifolds V of $\mathcal{K}^1$. We call F the free energy, too. Then

$$\mathcal{A} = \ dI\, F + \Psi \quad \text{on} \quad \mathcal{K}^1,$$

where Ψ on V has the form

$$\Psi(\xi)(\gamma) = S(s(\xi)) \cdot \ dI\, T(s(\xi)) \ \ \forall \xi \in V \subset \mathcal{K}^1 \text{ and } \forall \gamma \in A^1\left(S^1\mathbb{P}, \mathbb{R}^3\right)$$

dI is here the differential on $\mathcal{K}^1$.

We have considered here the thermodynamical setting only in the case of the virtual work done on $\mathbb{P}$. This can be easily generalized to the virtual work on the microstructure. To do this we define first the virtual work on the microstructure [4] and then we repeat the above argument.

References

[1] BAMBERG P. AND STERNBERG S., *A course in mathematics for students of phisic, II*, Cambridge University Press, Cambridge 1988.

[2] BINZ E., *On discrete media, their interaction forms and the origin of non-exactness of the virtual work*, in: "Symmetries in Science", (Eds. B. Gruber and M. Ramek), Plenum Press, New York 1997, 47–61.

[3] BINZ E., DE LEÓN M. AND SOCOLESCU D., *On a smooth geometric approach to the dynamics of media with microstructure*, C.R. Acad. Sci. Paris **326** IIb (1998), 227–232.

[4] BINZ E., DE LEÓN M. AND SOCOLESCU D., *Global dynamics of media with microstructure*, Extracta Math. **14** 2 (1999), 99–125.

[5] ECKMANN B., *Harmonische Funktionen und Randwertaufgaben in einem Komplex*, Comment. Math. Helv. **17** 2 (1944-45), 240–255.

[6] MAUGIN G.A., *The thermomechanics of nonlinear irreversible behaviours, An introduction*, World Scientific, New Jersey 1998.

[7] STRAUMANN E., *Thermodynamik*, Lecture Notes in Physics **265**, Springer, Berlin 1986.

AMS Subject Classification: 58F05, 73C50, 73Bxx, 80A10.

Ernst BINZ
Fakultät für Mathematik und Informatik
Universität Mannheim
68131 Mannheim, GERMANY
e-mail: `binz@math.uni-mannheim.de`

Dan SOCOLESCU
Fachbereich Mathematik
Universität Kaiserslautern
67663 Kaiserslautern, GERMANY
e-mail: `socolescu@mathematik.uni-kl.de`

between two cracks located at points x and ξ depends on both the radial and angular variables, and evolves with the current crack distribution pattern. Thus, the form of the influence function shall depend upon the distribution of the internal variables at each time / loading – step. The last integral is in fact a path integral, depending on the spatial distribution of the cracks. The path that do effectively contribute to the local stress increment on the left-hand side of (1) change according to the evolution of the spatial pattern of cracks.

In Ganghoffer et al., a path integral formulation of the nonlocal interactions has been formulated, with damage as a focus. The scalar damage variable there represents the internal variable. The new concepts advanced therein can be considered as an attempt to model in a phenomenological manner the nonlocal interactions between defects in a solid material. In this contribution, we only give the main thrust of the ideas developed in [7].

2. Path integral formulation of nonlocal mechanics

The formulation of nonlocal damage relies upon the thermodynamics of irreversi-ble processes; accordingly, a damage potential function is set up, with arguments the internal variables, namely the local and the nonlocal damage. The consistency condition for the damage potential function and its dependence upon the local and nonlocal damage imply an integro-differential equation for the rate of the local damage, that can be recast into the general form

$$\dot{d}(x) = \frac{1}{\int\limits_{\Omega} G_1(x, y)dy} \int\limits_{\Omega} G_1(x, y)\dot{d}(y)dy, \tag{2}$$

with $G_1(x, y)$ an influence function. Equality (2) is rewritten into the more compact form

$$\dot{d}(x) = G(x, y) \circ \dot{d}(y), \tag{3}$$

whereby the kernel G and the composition operator $\circ$ are identified from the integral form in (2), i.e. (3) defines an integral operator having the kernel

$$G(x, y) = \frac{1}{\int\limits_{\Omega} G_1(x, y)dy} G_1(x, y).$$

When the kernel $G(x, y)$ only depends on the difference $(x - y)$ (e.g. in the form of the gaussian (3)), equality (2) gives the rate of damage as the convolution product of the kernel with the rate of damage. From now on, the starting point shall be the relation (2), in which *we do not a priori know the kernel* $G(x, y)$. A path integration technique will then be used to determine the expression of this kernel.

Since the kernel G determines the evolution of the internal variable, it shall be called the *propagator* as well. Properties satisfied by the kernel G are first evidenced. First note that relation (3) embodies an implicit definition of G : elaborating (3) yields

$$\dot{d}(x) = G(x, y) \circ G(y, z) \circ \dot{d}(z) = G(x, z) \circ \dot{d}(z) \tag{4}$$

and therefore, one has formally

$$G(x, z) = G(x, y) \circ G(y, z) \tag{5}$$

in which the composition operator means that one first propagates the influence from x to y, and then from y to z. Relation (5) is called the *inclusion relation* of an intermediate point. In