# 5. Fracture mechanics from inter-atomic potentials

This section will be devoted to the study of a one-dimensional system of lattice interactions driven by some potentials that are usually involved in the description of atomic interactions. Examples of such potentials are Lennard-Jones potentials

$$J_{\rm LJ}(z) = \frac{c_1}{z^{12}} - \frac{c_2}{z^6},$$

with  $c_1, c_2 > 0$  and the restriction that z > 0, or Morse potentials

$$J_{\rm M}(z) = -cze^{-z},$$

with c > 0.

The common features of these potentials  $J : \mathbf{R} \to (-\infty, +\infty]$  are:

• the domain of J,  $\{z : J(z) < +\infty\}$ , is an interval, J admits a unique minimum point  $z^*$ , and on its domain J is (strictly) decreasing and convex for  $z \le z^*$  and (strictly) increasing for  $z \ge z^*$ ;

• J is smooth on its domain;

• J satisfies the growth conditions at  $\pm \infty$ :

$$\lim_{z \to -\infty} \frac{J(z)}{|z|} = +\infty, \qquad \lim_{z \to +\infty} J(z) = 0$$

 $(J_{\rm LJ}(z) \text{ is set equal to } +\infty \text{ for } z \leq 0).$ 

## 1 Nearest-neighbors

We consider energies of the form

$$\sum_{i=1}^{n} J(v_i - v_{i-1}), \qquad v : \{0, \dots, n\} \to \mathbf{R}$$

where  $n \in \mathbf{N}$ . For the sake of simplicity we consider a potential with the constraint that  $v_i - v_{i-1} \ge 0$  (for example, Lennard-Jones potentials). This will simplify some descriptions since the function v will always be non decreasing. To remove this constraint, it is sufficient to note that the growth condition at  $-\infty$  will provide strong compactness properties for the decreasing part of the function. Note that at this stage we have not performed any scaling of the energy.

### 1.1 A first scaling giving a trivial bulk energy

The first possibility is to perform the usual change of variables t0 interpret  $v_i - v_{i-1}$  as a difference quotient, and consider energies  $\varepsilon = \frac{1}{n}$ ,

$$E_{\varepsilon}(u) = \sum_{i=1}^{n} \varepsilon J\left(\frac{u_i - u_{i-1}}{\varepsilon}\right), \qquad u : \varepsilon \mathbf{Z} \cap [0, 1] \to \mathbf{R}$$

Note that if we consider simple problems of the form

$$m_{\varepsilon}(L) = \min\{E_{\varepsilon}(u) : u(0) = 0, u(1) = L\},\$$

then the monotonicity of test functions along with the fixed boundary conditions, provides a bound in BV(0, 1) of minimizers, and hence compactness in any  $L^p(0, 1)$   $(p < +\infty)$ ). We can then compute the  $\Gamma$ -limit of  $E_{\varepsilon}$  in  $L^1(0, 1)$  (or equivalently with respect to the weak<sup>\*</sup> convergence in BV(0, 1)). A trivial lower bound is obtained by identifying each u with its continuous piecewiseaffine interpolation and correspondingly the sum with an integral: if  $u_{\varepsilon} \to u$ 

$$\liminf_{\varepsilon} E_{\varepsilon}(u_{\varepsilon}) = \liminf_{\varepsilon} \int_0^1 J(u_{\varepsilon}') \, dt \ge \liminf_{\varepsilon} \int_0^1 J^{**}(u_{\varepsilon}') \, dt \ge \int_0^1 J^{**}(u') \, dt.$$

It must be noted that u is not AC, so that u' must be understood as the almost-everywhere defined derivative of u (that exists since u is non-decreasing). Note that u may be discontinuous (more precisely, it may have 'increasing' jumps), and that its discontinuities do not affect the value of the latter integral.

We have to check that this inequality is sharp. To this end note explicitly that

$$J^{**}(z) = \begin{cases} J(z) & \text{if } z \le z^* \\ J(z^*) & \text{if } z \ge z^* \end{cases}$$

and that a general  $u \in BV(0,1)$  may be approximated by  $u_k \in SBV(0,1)$  with a finite number of jumps and  $u' \leq z^*$  in such a way that

$$\lim_{k} \int_{0}^{1} J(u'_{k}) \, dt = \int_{0}^{1} J^{**}(u') \, dt.$$

It suffices then to consider  $u \in SBV(0,1)$ , with  $0 < u' \leq z^*$  and with a finite number of jumps. For these functions we may just take  $u_{\varepsilon} = u$  (more precisely, the discrete interpolation of u), and note that

$$E_{\varepsilon}(u_{\varepsilon}) = \sum_{i \in \{1, \dots, N\} \setminus I_{\varepsilon}^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + \sum_{i \in I_{\varepsilon}^*} \varepsilon J\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big),$$

where

$$I_{\varepsilon}^* = \{i : [\varepsilon(i-1), \varepsilon i) \cap S(u) \neq \emptyset\}$$

so that, for  $\varepsilon$  small enough,

$$E_{\varepsilon}(u_{\varepsilon}) = \sum_{i \in \{1,...,N\} \setminus I_{\varepsilon}^{*}} \varepsilon J\left(\frac{u_{i} - u_{i-1}}{\varepsilon}\right) + \sum_{i \in I_{\varepsilon}^{*}} \varepsilon J\left(\frac{u_{i} - u_{i-1}}{\varepsilon}\right)$$
  
$$\leq \sum_{i \in \{1,...,N\} \setminus I_{\varepsilon}^{*}} \varepsilon J\left(\frac{u_{i} - u_{i-1}}{\varepsilon}\right)$$
  
$$= \int_{0}^{1} J(u') dt + o(1),$$

as desired.

We must also note that if  $(u_{\varepsilon})$  is a sequence satisfying some boundary conditions; *e.g.*,  $u_{\varepsilon}(0) = 0, u_{\varepsilon}(1) = L$ , then the limit function for this energy may not satisfy these conditions.

Anyhow, since each one of these  $u_{\varepsilon}$  is increasing we deduce that we have  $u(0+) \ge 0$  and  $u(1-) \le L$  $(u(t\pm))$  are the traces of u at the point t). For such u the construction above still works unchanged.

As a consequence of this  $\Gamma$ -convergence result, we obtain that the limit of  $m_{\varepsilon}(L)$  is given by

$$m(L) = \min\{\int_0^1 J^{**}(u') \, dt : u \text{ increasing, } u(0+) \ge 0, \ u(1-) \le L\} = J^{**}(L)$$

The information we can draw from this minimum problem is that we have two types of regimes corresponding to the case:

• if  $L \leq z^*$  then the unique minimizer of m(L) is the linear function u(t) = Lt;

• if  $L > z^*$  then every increasing function with  $u' \ge z^*$ ,  $u(0+) \ge 0$  and  $u(1-) \le L$  is a minimizer for m(L).

If we interpret our system as a chain of atoms, then we may interpret the corresponding continuous model as having an elastic behavior in a *compressive* regime  $(z \leq z^*)$ , while it undergoeas complete failure in a *tensile* regime  $(z > z^*)$ .

It must be noted that our result is in a sense 'trivial', as it says that  $E_{\varepsilon}$  can be identified with the integral

$$\int_0^1 J(u') \, dt,$$

whose relaxation is precisely  $\int_0^1 J^{**}(u') dt$ .

### 1.2 A second scaling giving Griffith fracture energy

We first perform a translation of the energy, by setting

$$\psi(z) = J(z + z^*) - J(z^*),$$

so that the minimum of  $\psi$  is  $\psi(0) = 0$ . We then perform a different scaling of the energies, whose underlying idea is to have the bulk and interfacial energy of the same order.

The energies we consider are now

$$E_{\varepsilon}(u) = \sum_{i=1}^{N} \psi\left(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\right)$$

The choice of this scaling is heuristically explained as follows: if u is (the interpolation of) a smooth function, then

$$\psi\Big(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\Big) = \psi\Big(\sqrt{\varepsilon}\frac{u_i - u_{i-1}}{\varepsilon}\Big) \approx \psi(\sqrt{\varepsilon}u'(\varepsilon i)) \approx \varepsilon \frac{1}{2}\psi''(0)(u'(\varepsilon i))^2;$$

here and after we make the assumption that

$$\alpha := \frac{1}{2}\psi''(0) > 0. \tag{1}$$

In this way we have

$$E_{\varepsilon}(u) \approx \alpha \int_0^1 |u'|^2 dt.$$

Conversely, if we only have (increasing) jumps (*i.e.*, u is piecewise constant and non-decreasing), then if  $t \in S(u) \cap [\varepsilon(i-1), \varepsilon_i]$  we have

$$\psi\left(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\right) \approx \psi\left(\frac{u^+(t) - u^-(t)}{\sqrt{\varepsilon}}\right) \approx \psi(+\infty) = -J(z^*) =: \beta,$$

and

 $E_{\varepsilon}(u) \approx \beta \#(S(u)).$ 

Actually, what we have just shown (to have a complete proof it suffices to use a density argument by functions that are smooth except for a finite numbers of increasing jumps) is that we have an upper bound with the functional, whose domain are SBV functions with only a finite number of increasing jumps, given by

$$F(u) = \alpha \int_0^1 |u'|^2 dt + \beta \#(S(u)) \qquad (u^+ > u^- \text{ on } S(u)).$$

We now show that this is also a lower bound. To do this, we compare our energy with a family of energies whose limit is easier to compute, and subsequently optimize this estimate. The family  $\mathcal{F}$  of energy densities we consider are all  $f \leq \psi$  of the form

$$f(z) = \begin{cases} c_1 |z|^2 \wedge c_3 & \text{if } z \le 0\\ c_1 |z|^2 \wedge c_2 & \text{if } z \ge 0 \end{cases}$$

with  $c_i > 0$ ; *i.e.* f is a 'non-symmetrically-truncated quadratic potential'.

Note that

$$\sup\{c_1 : f \in \mathcal{F}\} = \alpha, \quad \sup\{c_2 : f \in \mathcal{F}\} = \beta, \quad \sup\{c_3 : f \in \mathcal{F}\} = +\infty.$$
(2)

Note also that

$$f\left(\frac{u_i - u_{i-1}}{\sqrt{\varepsilon}}\right) = \begin{cases} c_3 & \text{if } \frac{u_i - u_{i-1}}{\varepsilon} \le -\sqrt{\frac{c_3}{c_1}} \frac{1}{\sqrt{\varepsilon}} \\ \varepsilon c_1 \left| \frac{u_i - u_{i-1}}{\varepsilon} \right|^2 & \text{if } -\sqrt{\frac{c_3}{c_1}} \frac{1}{\sqrt{\varepsilon}} < \frac{u_i - u_{i-1}}{\varepsilon} < \sqrt{\frac{c_2}{c_1}} \frac{1}{\sqrt{\varepsilon}} \\ c_2 & \text{if } \frac{u_i - u_{i-1}}{\varepsilon} \ge \sqrt{\frac{c_2}{c_1}} \frac{1}{\sqrt{\varepsilon}}. \end{cases}$$
(3)

Let  $(u_{\varepsilon})$  be a sequence converging to some u. Then we identify each  $u_{\varepsilon}$  with its piecewise-affine discontinuous interpolation  $v_{\varepsilon}$  with discontinuity set  $S(v_{\varepsilon}) = S_{\varepsilon}^+ \cup S_{\varepsilon}^-$ , where

$$S_{\varepsilon}^{+} = \{\varepsilon i : \frac{u_{\varepsilon}(\varepsilon i) - u_{\varepsilon}(\varepsilon(i-1))}{\sqrt{\varepsilon}} \ge \sqrt{\frac{c_2}{c_1}}\}, \qquad S_{\varepsilon}^{-} = \{\varepsilon i : \frac{u_{\varepsilon}(\varepsilon i) - u_{\varepsilon}(\varepsilon(i-1))}{\sqrt{\varepsilon}} \le -\sqrt{\frac{c_3}{c_1}}\},$$

and  $v_{\varepsilon}$  is constant on the corresponding intervals  $(\varepsilon(i-1), \varepsilon i)$ .

We then have

$$\begin{split} \liminf_{\varepsilon} E_{\varepsilon}(u_{\varepsilon}) &= \liminf_{\varepsilon} F_f(v_{\varepsilon}) \\ &=: \liminf_{\varepsilon} \left( c_1 \int_0^1 |v_{\varepsilon}'|^2 \, dt + c_2 \# (S^+(v_{\varepsilon})) + c_3 \# (S^-(v_{\varepsilon})) \right) \\ &\geq c_1 \int_0^1 |u'|^2 \, dt + c_2 \# (S^+(u)) + c_3 \# (S^-(u)), \end{split}$$

where

$$S^+(v) := \{ t \in S(u) : u^+ > u^- \}, \qquad S^-(v) := \{ t \in S(u) : u^+ < u^- \}.$$

We have used the lower semicontinuity of  $F_f$ .

We can locally optimize this estimate; *i.e.*, we may take the supremum in  $c_1, c_2, c_3$  separately. Taking the supremum in  $c_3$  implies that  $S^-(u) = \emptyset$ , while the other two 'optimizations' give the desired lower bound.

This new scaling approximates minimum boundary value problems for  $E_{\varepsilon}$  with

$$\begin{split} m(L) &= \min\{\alpha \int_0^1 |u|^2 \, dt + \beta \#(\widetilde{S}(u)) : u^+ > u^-, \ u(0^+) \ge 0, u(1-) \le L\} \\ &= \begin{cases} \min\{\alpha L^2, \beta\} & \text{if } L \ge 0\\ \alpha L^2 & \text{if } L < 0, \end{cases} \end{split}$$

where we take into account that the jump of u may occur at the boundary, setting

$$\widetilde{S}(u) = S(u) \cup \{t \in \{0, 1\} : \widetilde{u}^-(t) < \widetilde{u}^+(t)\},\$$

 $\tilde{u}^- = u^-$  on (0,1],  $\tilde{u}^+ = u^+$  on [0,1),  $\tilde{u}^-(0) = 0$  and  $\tilde{u}^+(1) = L$ .

The case  $L \ge 0$  corresponds to the tensile regime in the previous scaling, and the corresponding energy may be interpreted as a *Griffith fracture energy*.

Note that for  $m(L) = \beta$  we have infinitely many minimizers given by

$$u(t) = \begin{cases} 0 & \text{if } t \le t_0 \\ L & \text{if } t > t_0; \end{cases}$$

*i.e.*, the fracture site is not localized.

# 2 Next-to-nearest neighbors

We now consider energies taking into account first and second neighbors; *i.e.*, both terms of the form  $J(u_i - u_{i-1})$  and of the form  $J(u_{i+1} - u_{i-1})$ .

In this case, the way boundary conditions are stated does influence the form of the limit problems. Dirichlet boundary conditions

$$u(0) = 0, \qquad u(1) = L$$

may be imposed as a pointwise condition on 0 and 1, or by requiring that u be a periodic perturbation of the linear function  $u_L(t) = Lt$ . In terms of minimum problems, in the first case we consider

$$\min\left\{\sum_{i=1}^{N} J(u_i - u_{i-1}) + \sum_{i=1}^{N-1} J(u_{i+1} - u_{i-1}) : u_0 = 0, \ u_N = L\right\}$$

(note that we have N nearest-neighbor interactions and N-1 next-to-nearest neighbor interactions in the interval  $0, \ldots, N$ ), while in the second one

$$\min\left\{\sum_{i=1}^{N} \left(J(u_i - u_{i-1}) + J(u_{i+1} - u_{i-1})\right) : u_0 = 0, \ u_N = L, u_{N+1} = u_1 + L\right\}$$

(equivalently, this minimum is performed among  $u : \mathbb{Z} \to \mathbb{R}$  satisfying the periodicity condition  $u_{i+N} = u_i + L$ ).

### 2.1 First scaling

In this case boundary conditions given in either way give the same limit energy. We briefly illustrate the result in a more general case, for energies of the form

$$E_{\varepsilon}(u) = \sum_{i=1}^{N} \varepsilon \Big( J_1\Big(\frac{u_i - u_{i-1}}{\varepsilon}\Big) + J_2\Big(\frac{u_{i+1} - u_{i-1}}{\varepsilon}\Big) \Big),$$

where  $J_1, J_2$  satisfy the same conditions as the Lennard-Jones potentials.

The idea is to rewrite the energy in a more symmetric way as

$$E_{\varepsilon}(u) = \sum_{i=1}^{N} \varepsilon \left( \frac{1}{2} J_1\left(\frac{u_i - u_{i-1}}{\varepsilon}\right) + \frac{1}{2} J_1\left(\frac{u_{i+1} - u_i}{\varepsilon}\right) + J_2\left(\frac{u_{i+1} - u_{i-1}}{\varepsilon}\right) \right).$$

then to integrate out the nearest-neighbor interactions by considering

$$\tilde{J}(z) = \frac{1}{2} \min\{J(z_1) + J(z_2) : z_1 + z_2 = z\},\$$

and the 'effective energy density'

$$J_{\text{eff}}(z) = J_2(2z) + \tilde{J}(2z).$$

Note that

$$\left(\frac{1}{2}J_1\left(\frac{u_i-u_{i-1}}{\varepsilon}\right) + \frac{1}{2}J_1\left(\frac{u_{i+1}-u_i}{\varepsilon}\right) + J_2\left(\frac{u_{i+1}-u_{i-1}}{\varepsilon}\right) \right)$$

$$\geq \left(\tilde{J}\left(\frac{u_{i+1}-u_i}{\varepsilon}\right) + J_2\left(\frac{u_{i+1}-u_i}{\varepsilon}\right) \right) = J_{\text{eff}}\left(\frac{u_{i+1}-u_{i-1}}{2\varepsilon}\right).$$

In this way we have the inequality

$$E_{\varepsilon}(u) \geq \sum_{i=1}^{N} \varepsilon J_{\text{eff}} \left( \frac{u_{i+1} - u_{i-1}}{2\varepsilon} \right) \\ = \frac{1}{2} \left( \sum_{i \text{ even}} 2\varepsilon J_{\text{eff}} \left( \frac{u_{i+1} - u_{i-1}}{2\varepsilon} \right) + \sum_{i \text{ odd}} 2\varepsilon J_{\text{eff}} \left( \frac{u_{i+1} - u_{i-1}}{2\varepsilon} \right) \right),$$

and hence a lower bound is given by

$$F(u) = \int_0^1 (J_{\text{eff}})^{**}(u') \, dt.$$

This is indeed the  $\Gamma$ -limit.

In the Lennard-Jones case

$$J_1(z) = J_2(z) = J(z)$$

the recovery sequences are simple discrete interpolations and we indeed have

$$J_{\text{eff}}(z) = J(z) + J(2z),$$

that is an energy again of Lennard-Jones type. Note that the critical state  $z^*$  giving the transition between the compressive and tensile regions is then defined as the minimizer of  $J_{\text{eff}}$ .

### 2.2 Second scaling. Periodic case

The first scaling has served in finding the minimal state  $z^*$ . Now we may scale differently the energies by setting

$$E_{\varepsilon}(u) = \sum_{i=1}^{N} \left( \frac{1}{2} J \left( \frac{u_i - u_{i-1}}{\sqrt{\varepsilon}} + z^* \right) + \frac{1}{2} J \left( \frac{u_{i+1} - u_i}{\sqrt{\varepsilon}} + z^* \right) + J \left( \frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^* \right) - J_{\text{eff}}(z^*) \right).$$

A first lower bound is then obtained by the inequality

$$E_{\varepsilon}(u) \ge \sum_{i=1}^{N} J_{\text{eff}}\left(\frac{u_{i+1} - u_{i-1}}{\sqrt{\varepsilon}} + 2z^*\right)$$

The right-hand side is a superposition of two lattice energies and gives the  $\Gamma$ -limit

$$F_0(u) = \alpha \int_0^1 |u'|^2 dt + C \#(S(u)),$$

where

$$\alpha := \frac{1}{2} J_{\text{eff}}''(z^*) = \frac{1}{2} J''(z^*) + 2J''(2z^*), \qquad C := \frac{1}{2} \min J - \min J_{\text{eff}} = J_{\text{eff}}(+\infty) - \min J_{\text{eff}}.$$

This lower bound is also an upper bound if  $u \in H^1(0,1)$ ; *i.e.*, if  $S(u) = \emptyset$ . Indeed, if u is smooth then a recovery sequence is simply its discrete interpolation  $u_{\varepsilon}$  for which

$$E_{\varepsilon}(u_{\varepsilon}) \approx \sum_{i=1}^{N} (J(\sqrt{\varepsilon}u'(\varepsilon i) + z^{*}) + J(2\sqrt{\varepsilon}u'(\varepsilon i) + 2z^{*}) - J_{\text{eff}}(z^{*}))$$
$$\approx \sum_{i=1}^{N} (J_{\text{eff}}(\sqrt{\varepsilon}u'(\varepsilon i) + z^{*}) - J_{\text{eff}}(z^{*}))$$
$$\approx \sum_{i=1}^{N} \alpha \varepsilon |u'(\varepsilon i)|^{2} \approx \alpha \int_{0}^{1} |u'|^{2} dt.$$

In general the lower bound above is not optimal for jumps. Indeed, suppose that we have one jump (that in this periodic setting we may always suppose at 0); *i.e.*,  $u_{\varepsilon}(0) = 0$ ,  $u_{\varepsilon}(\varepsilon) \approx u(0+) = c > 0$ , then

$$\begin{split} E_{\varepsilon}(u) &= \left(\frac{1}{2}J\left(\frac{u_{1}}{\sqrt{\varepsilon}}+z^{*}\right)+\frac{1}{2}J\left(\frac{u_{2}-u_{1}}{\sqrt{\varepsilon}}+z^{*}\right)+J\left(\frac{u_{2}-u_{0}}{\sqrt{\varepsilon}}+2z^{*}\right)-J_{\text{eff}}(z^{*})\right) \\ &+\sum_{i=2}^{N-1}\left(\frac{1}{2}J\left(\frac{u_{i}-u_{i-1}}{\sqrt{\varepsilon}}+z^{*}\right)+\frac{1}{2}J\left(\frac{u_{i+1}-u_{i}}{\sqrt{\varepsilon}}+z^{*}\right)+J\left(\frac{u_{i+1}-u_{i-1}}{\sqrt{\varepsilon}}+2z^{*}\right)-J_{\text{eff}}(z^{*})\right) \\ &+\left(\frac{1}{2}J\left(\frac{-u_{N-1}}{\sqrt{\varepsilon}}+z^{*}\right)+\frac{1}{2}J\left(\frac{u_{1}}{\sqrt{\varepsilon}}+z^{*}\right)+J\left(\frac{u_{1}-u_{N-1}}{\sqrt{\varepsilon}}+2z^{*}\right)-J_{\text{eff}}(z^{*})\right) \\ &\approx \frac{1}{2}J\left(\frac{u_{2}-u_{1}}{\sqrt{\varepsilon}}+z^{*}\right)-J_{\text{eff}}(z^{*}) \\ &+\sum_{i=2}^{N-1}\left(\frac{1}{2}J\left(\frac{u_{i}-u_{i-1}}{\sqrt{\varepsilon}}+z^{*}\right)+\frac{1}{2}J\left(\frac{u_{i+1}-u_{i}}{\sqrt{\varepsilon}}+z^{*}\right)+J\left(\frac{u_{i+1}-u_{i-1}}{\sqrt{\varepsilon}}+2z^{*}\right)-J_{\text{eff}}(z^{*})\right) \end{split}$$

$$+\frac{1}{2}J\left(\frac{u_N-u_{N-1}}{\sqrt{\varepsilon}}+z^*\right)+J\left(\frac{u_1-u_{N-1}}{\sqrt{\varepsilon}}+2z^*\right)-J_{\text{eff}}(z^*)$$

$$\geq 2\inf\left\{\frac{1}{2}J(z^*+z_1)+\sum_{i=1}^{K}\left(\frac{1}{2}J(z_i+z^*)+\frac{1}{2}J(z_{i+1}+z^*)+J(2z^*+z_i+z_{i+1})\right\}-2J_{\text{eff}}(z^*)\right\}$$

where K is any fixed natural number ( $\leq N/2$ ). The optimal lower bound for a jump is then given by

$$\beta := 2B - 2\min J_{\text{eff}},$$

where

$$B := \inf_{K} \inf \left\{ \frac{1}{2} J(z^* + z_1) + \sum_{i=1}^{K} \left( \frac{1}{2} J(z_i + z^*) + \frac{1}{2} J(z_{i+1} + z^*) + J(2z^* + z_i + z_{i+1}) \right) \right\}$$

We may interpret B as a free-boundary energy: the energy to generate a discontinuity amounts to the energy  $-2 \min J_{\text{eff}}$  (that is positive) due to the complete detachment of the neighboring atoms plus the energy 2B (that is negative) due to the rearrangements of the atoms on both sides of the fracture.

Finally, the  $\Gamma$ -limit is again given by

$$F(u) = \alpha \int_0^1 |u'|^2 \, dt + \beta \#(S(u))$$

### 2.3 Second scaling. Boundary terms

In this case, the  $\Gamma$ -limit for the integral term and for interior jumps is the same, while the estimate as above performed for a jump at the boundary gives  $B - \min J_{\text{eff}} = \beta/2$ ; hence, the resulting limit energy is

$$F(u) = \alpha \int_0^1 |u'|^2 dt + \beta \#(S(u)) + \frac{\beta}{2} \#(\widetilde{S(u)}) \cap \{0, 1\}).$$

As a consequence we have a *localization at the boundary* of the discontinuity points.

### References

- [1] A. Braides, Γ-convergence for Beginners, Oxford University Press, Oxford, 2002.
- [2] A.Braides, A.J.Lew and M.Ortiz. Effective cohesive behavior of layers of interatomic planes. Archive Rational Mech. Anal., to appear
- [3] L. Truskinovsky, Fracture as a phase transition, Contemporary research in the mechanics and mathematics of materials (R.C. Batra and M.F. Beatty eds.) CIMNE, Barcelona, 1996, 322-332.