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J. Phys. A: Math. Gen. **38** (2005) 4337–4347 doi:10.1088/0305-4470/38/20/003

Hyperbolicity, convexity and shock waves in one-dimensional crystalline solids

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Received 11 January 2005, in final form 24 March 2005
Published 3 May 2005
Online at stacks.iop.org/JPhysA/38/4337

Abstract
For a continuum model of one-dimensional anharmonic crystal lattices at finite temperatures, which was derived from a statistical-mechanical model proposed recently, we clarify the classification of its differential system. That is, we determine not only the strict hyperbolicity and convexity regions but also the elliptic and parabolic regions in the space of the state. The melting point is found to be on the boundary of the convexity region. Then we derive the Rankine–Hugoniot relations, and we prove that the admissible shocks are always in the stable region of convexity.

PACS numbers: 05.70.Ln, 46.05.+b, 47.40.Sn, 61.50.Ah

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The entropy principle plays a fundamental role in thermodynamics of continua. In fact it provides a powerful constraint in order to select the physical constitutive equations in the case of classical solutions, and for hyperbolic theories it becomes a fruitful selection rule for admissible weak solutions [1, 2]. Furthermore, if the principle is combined with the stability requirement of the concavity of the entropy density in the thermodynamical context or the convexity of energy in the mechanical or electrodynamic case, it permits us to rewrite the field equations in the form of a symmetric hyperbolic system through the introduction of the privileged main field components [3–5].

On the other hand, in nonlinear theories the hyperbolicity and in particular the concavity of the entropy density may be valid only in some region of state variables. Typical examples are the nonlinear elasticity in which the full concavity is in contrast to the objectivity principle if the deformation is large. And the concavity is true only for sufficiently small deformations in a neighbourhood of the undeformed configuration [6] (see also [1]); in nonlinear electrodynamics of Born and Infeld in which the convexity of energy remains verified if the electric field is less than a limit value [4]. Another interesting case is that of extended thermodynamics in which the hyperbolicity and the concavity are verified only in a neighbourhood of an equilibrium state [7].

The knowledge of the hyperbolicity region is mandatory to check the admissibility of the solutions and the corresponding boundary and Cauchy data. Moreover the convexity[3] is a necessary condition for the well posedness of the Cauchy problem (local in time) [1, 8, 9].

In the first part of this paper we will study the classification of the differential system for a continuum model of one-dimensional anharmonic crystal lattices at finite temperatures [10]. The model takes thermal vibration of constituent atoms into account explicitly, and it was derived from a nonequilibrium statistical-mechanical model of crystal lattices with a continuum approximation. As is well known, crystal lattices have been a good physical model to study nonlinear waves propagating in solids [11]. We will clarify several interesting features from both mathematical and physical points of view; that is, we will prove that there exist several regions in the state space across which the system of equations changes its differential structure: a region in which the system is strictly hyperbolic and regions in which the system is parabolic or elliptic. The region in which the convexity holds and the system is symmetric hyperbolic is, according to the general theory, a subset of the strictly hyperbolic region. Thermodynamically stable states are always in the convexity region, a definition of which will be given below, except for the limiting case, i.e. the melting point, which is on the boundary of the convexity region.

In the second part of the paper we will study shock waves in the crystalline solids, and we will prove that the admissibility Lax conditions guarantee that all the Rankine–Hugoniot curves give rise to processes in the convexity region.

2. System of differential equations for crystalline solids

We here briefly summarize the field equations for the continuum model of one-dimensional anharmonic crystal lattices at finite temperatures [10] with atomic mass M, lattice constant a_e, and interatomic potential given by the Morse function

$$\phi(x) = D(\mathrm{e}^{-2\alpha(x-r_0)} - 2\,\mathrm{e}^{-\alpha(x-r_0)}),$$

where D, α and r_0 are material constants [12, 13].

The variables in the field equations are the dimensionless quantities $d(X,t)$, $q(X,t)$, $g(X,t)$ and $r(X,t)$ defined below. Here X is the position of a material point in the reference configuration, and t is the time. As the reference configuration the thermal equilibrium state at absolute temperature T with no external force and no translation motion is adopted. The physical meaning of the four quantities mentioned above can be understood easily from their definitions [10, 14]:

$$\begin{aligned}
&\frac{\partial}{\partial X}\langle h(X,t)\rangle \equiv (\alpha a_e)^{-1} d(X,t), \qquad \frac{\partial}{\partial t}\langle h(X,t)\rangle \equiv \sqrt{\frac{D}{M}}\,q(X,t),\\
&\langle [h(X,t) - \langle h(X,t)\rangle]^2\rangle \equiv \alpha^{-2}[\lambda + g(X,t)],\\
&\left\langle \left[\frac{\partial}{\partial t}(h(X,t) - \langle h(X,t)\rangle)\right]^2 \right\rangle \equiv \frac{D}{M}\left[\frac{k_B T}{D} + r(X,t)\right],
\end{aligned} \tag{1}$$

[3] In what follows we will always refer to the convexity with the usual convention to consider, in the thermodynamical case, the entropy density changed in sign.

where $\langle\ \rangle$ stands for a statistical average over the non-equilibrium distribution function, $h(X,t)$ is the displacement of a constituent atom from its thermal equilibrium point X and k_B is the Boltzmann constant. The quantity λ is the reduced mean square displacement due to the thermal vibration in the reference equilibrium state

$$\lambda = \alpha^2 \langle [h(X,t)]^2 \rangle_{\text{equilibrium}}$$

which is related to the temperature T such that [14]

$$\frac{k_B T}{4D} = \lambda\, \mathrm{e}^{-2\lambda}.$$

The field equations, that is, the conservation laws of mass, momentum and energy, are summarized as follows:

$$\begin{aligned} &\Omega^{-1}\frac{\partial d}{\partial t} - a_e \frac{\partial q}{\partial X} = 0, \\ &\Omega^{-1}\frac{\partial q}{\partial t} + a_e \frac{\partial \pi}{\partial X} = 0, \\ &\Omega^{-1}\frac{\partial \varepsilon}{\partial t} + a_e \frac{\partial q\pi}{\partial X} = 0, \end{aligned} \tag{2}$$

where Ω is a microscopic characteristic frequency of atomic vibration defined by

$$\Omega = \alpha\sqrt{\frac{D}{M}}.$$

The dimensionless pressure π and the dimensionless energy density ε are given by

$$\begin{aligned} \pi &= 2\mathrm{e}^{-2\lambda}(\mathrm{e}^{4g-2d} - \mathrm{e}^{g-d}), \\ \varepsilon &= \frac{1}{2}\left(\frac{k_B T}{D} + q^2 + r\right) + \mathrm{e}^{-2\lambda}(\mathrm{e}^{4g-2d} - 2\mathrm{e}^{g-d}) = \frac{1}{2}q^2 + u, \end{aligned} \tag{3}$$

with u being dimensionless internal energy density.

In addition to the field equations, there exists an equation of state [10] such that

$$r = 4\mathrm{e}^{-2\lambda}(\lambda + g)(2\mathrm{e}^{4g-2d} - \mathrm{e}^{g-d}) - 4\lambda\,\mathrm{e}^{-2\lambda}. \tag{4}$$

By using this equation we may eliminate the quantity r in the quantities ε and u.

In the following it is convenient to introduce the new variables:

$$\psi = \mathrm{e}^{-2d+4g}; \qquad j = \frac{2}{\psi}\,\mathrm{e}^{-d+g}; \qquad \widehat{g} = g + \lambda; \tag{5}$$

($\widehat{g} \geqslant 0$ from $(1)_3$). Then from (3) and (4) we have

$$\begin{aligned} &\pi = \mathrm{e}^{-2\lambda}\psi(2 - j); \qquad \varepsilon = \frac{1}{2}\left(\frac{k_B T}{D} + q^2 + r\right) + \mathrm{e}^{-2\lambda}\psi(1 - j); \\ &r = \mathrm{e}^{-2\lambda}(-4\lambda + 2\widehat{g}\psi(4 - j)). \end{aligned}$$

3. Hyperbolicity region

System (2) is a particular case of a system of conservation laws

$$\frac{\partial \mathbf{F}(\mathbf{u})}{\partial t} + \frac{\partial \mathbf{G}(\mathbf{u})}{\partial X} = 0 \tag{6}$$

through the identification

$$\mathbf{F}(\mathbf{u}) \equiv \begin{pmatrix} d \\ q \\ \varepsilon \end{pmatrix}, \qquad \mathbf{G}(\mathbf{u}) \equiv a_e \Omega \begin{pmatrix} -q \\ \pi \\ q\pi \end{pmatrix},$$

and choosing for example as field variables:

$$\mathbf{u} \equiv \begin{pmatrix} d \\ q \\ g \end{pmatrix}.$$

As is well known, system (6) is hyperbolic in time direction if the associated eigenvalue problem

$$(\mathbf{B}(\mathbf{u}) - v\mathbf{A}(\mathbf{u}))\mathbf{d} = 0; \qquad \mathbf{A}(\mathbf{u}) = \nabla_{\mathbf{u}}\mathbf{F}(\mathbf{u}), \qquad \mathbf{B}(\mathbf{u}) = \nabla_{\mathbf{u}}\mathbf{G}(\mathbf{u}) \tag{7}$$

admits real eigenvalues v (characteristic velocities) and a set of linearly independent eigenvectors $\mathbf{d}$. In the case of acceleration waves the jump of the normal derivative across the wave front is proportional to the right eigenvector, and a disturbance propagates with the characteristic velocity [4, 15]. It is possible to obtain (7) from (6) through the formal chain rule of operators,

$$\frac{\partial}{\partial t} \to -v\delta, \qquad \frac{\partial}{\partial X} \to \delta,$$

that have the advantage of not requiring the explicit expression for the matrices $\mathbf{A}$ and $\mathbf{B}$. With these symbols $\delta\mathbf{u}$ identifies with the right eigenvector.

Let us introduce the dimensionless characteristic velocity

$$w = \frac{v}{a_e\Omega};$$

then from equation $(2)_1$ we obtain

$$\delta q = -w\delta d \tag{8}$$

while from $(2)_2$ taking into account (8)

$$\delta g = \mathrm{e}^{2\lambda}w^2 + (j-4)\psi; \qquad \delta d = (j-8)\psi. \tag{9}$$

Finally from $(2)_3$ we obtain the characteristic velocities:

$$w = 0; \qquad w^2 = \frac{-2\mathrm{e}^{-2\lambda}\psi}{(2+\widehat{g})}\frac{(j-j_1)(j-j_2)}{j-j_3}, \tag{10}$$

where

$$\begin{aligned} j_1 &= 4 + \widehat{g} - \sqrt{\widehat{g}(8+\widehat{g})}, \\ j_2 &= 4 + \widehat{g} + \sqrt{\widehat{g}(8+\widehat{g})}, \\ j_3 &= 8\frac{1+2\widehat{g}}{2+\widehat{g}}. \end{aligned} \tag{11}$$

Therefore the three right eigenvectors are given such that

$$\mathbf{d} \equiv \begin{pmatrix} (j-8)\psi \\ -w(j-8)\psi \\ \mathrm{e}^{2\lambda}w^2 + (j-4)\psi \end{pmatrix}, \tag{12}$$

where w is one of the three roots of (10).

From (10) and (11) it is easy to see that the strict hyperbolicity region (distinct characteristic velocities) is the following region of the plane $\{\widehat{g}, j\}$:

$$\mathcal{D}_h : \{j < j_1 \forall \widehat{g}, \text{ or } j_3 < j < j_2 \text{ and } \widehat{g} \neq 1\}, \tag{13}$$

see figure 1.

For $j = j_2$, or $j = j_1$, we have $w = 0$; i.e. we have a triple eigenvalue and strict hyperbolicity is lost but the system also loses the hyperbolicity because in this case we do not have a set of linearly independent eigenvectors (see (12)).

For $j \to j_3$ and $\widehat{g} \neq 1$, $w \to \infty$ and the system becomes parabolic.

In the other regions the system has complex eigenvalues and therefore has elliptic behaviour.

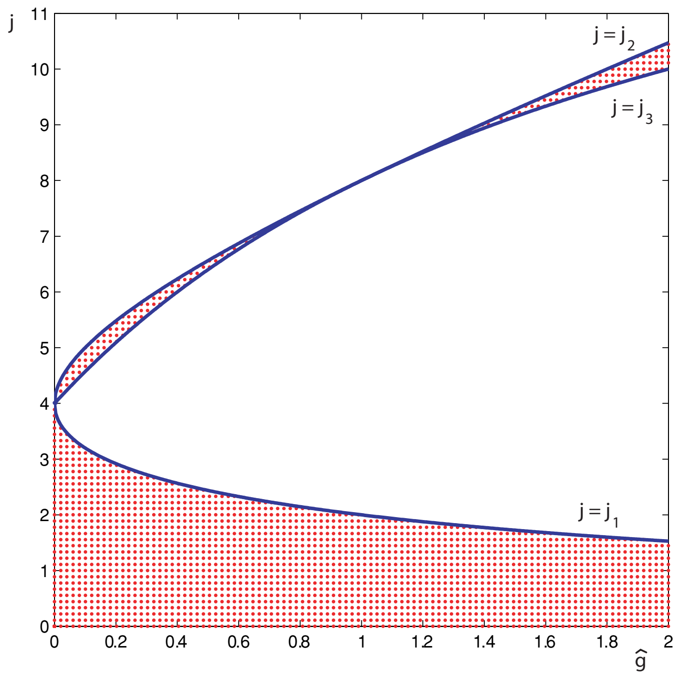

Figure 1. Hyperbolicity domain (grey region) in the state space $(\hat{g}, j)$.

4. Symmetric hyperbolic system and convexity region

It is easy to verify that all classical solutions of system (2) also satisfy the balance of entropy

$$\frac{\partial S}{\partial t} = 0, \tag{14}$$

where the entropy density is given by [10]

$$S = \frac{k_B}{2} \ln \left\{ 1 + \frac{1}{\lambda} \left(\frac{e^{2\lambda}}{4} r + g \right) + \frac{e^{2\lambda}}{4\lambda^2} g r \right\}.$$

Therefore the differential system (2) and the entropy law (14) belong to the general theory of systems of conservation laws (6) with a supplementary law

$$\frac{\partial h(\mathbf{u})}{\partial t} + \frac{\partial k(\mathbf{u})}{\partial X} = 0$$

with, in the present case,

$$h = -\frac{S}{k_B}; \qquad k = 0.$$

In this case, it is well known [3–5] that system (6) can be rewritten as a symmetric hyperbolic system in the sense of Friedrichs provided that we choose as field variables the main field

$$\mathbf{u}' = \frac{\partial h(\mathbf{u})}{\partial \mathbf{u}}; \qquad \mathbf{u} \equiv \mathbf{F} \tag{15}$$

and that h is a convex function of $\mathbf{u}$. In fact it is possible to introduce the Legendre transform of h,

$$h' = \mathbf{u}' \cdot \mathbf{u} - h,$$

and the potential

$$k' = \mathbf{u}' \cdot \mathbf{G} - k$$

such that we have

$$\mathbf{u} = \frac{\partial h'(\mathbf{u}')}{\partial \mathbf{u}'}; \qquad \mathbf{G} = \frac{\partial k'(\mathbf{u}')}{\partial \mathbf{u}'}. \tag{16}$$

Therefore taking into account (16), system (6) (with $\mathbf{u} \equiv \mathbf{F}$) becomes

$$\mathbf{A}'(\mathbf{u}')\frac{\partial \mathbf{u}'}{\partial t} + \mathbf{B}'(\mathbf{u}')\frac{\partial \mathbf{u}'}{\partial X} = 0$$

with

$$\mathbf{A}'(\mathbf{u}') = \frac{\partial^2 h'(\mathbf{u}')}{\partial \mathbf{u}' \partial \mathbf{u}'} \qquad \text{symmetric and positive definite}$$

and

$$\mathbf{B}'(\mathbf{u}') = \frac{\partial^2 k'(\mathbf{u}')}{\partial \mathbf{u}' \partial \mathbf{u}'} \qquad \text{symmetric.}$$

The symmetric systems have very good properties concerning the qualitative analysis. In fact the Cauchy (local in time) problem is well posed [1, 8, 9]. Therefore the crucial point of this technique is to evaluate the main field and then to verify the convexity of h with respect to $\mathbf{u}$, or equivalently the convexity of the Legendre transform h' with respect to the dual field $\mathbf{u}'$. For that it is sufficient to verify that the quadratic form

$$Q = \delta \mathbf{u}' \cdot \delta \mathbf{u}$$

is positive definite.

In fact from (15) and (16) we have

$$Q = \delta \mathbf{u}' \cdot \delta \mathbf{u} = \delta \left(\frac{\partial h(\mathbf{u})}{\partial \mathbf{u}} \right) \cdot \delta \mathbf{u} = \delta \mathbf{u}^T \frac{\partial^2 h(\mathbf{u})}{\partial \mathbf{u} \partial \mathbf{u}} \delta \mathbf{u} > 0, \qquad \forall\, \delta \mathbf{u} \neq 0$$

or

$$Q = \delta \mathbf{u}' \cdot \delta \mathbf{u} = \delta \mathbf{u}' \cdot \delta \left(\frac{\partial h'(\mathbf{u}')}{\partial \mathbf{u}'} \right) = \delta \mathbf{u}' \frac{\partial^2 h'(\mathbf{u}')}{\partial \mathbf{u}' \partial \mathbf{u}'} \delta \mathbf{u}'^T > 0, \qquad \forall\, \delta \mathbf{u}' \neq 0.$$

Now as we mentioned in the introduction there exist physical cases in which the convexity does not hold for all the values of the field variables. In this case it is very important to establish the domain of the convexity because the boundary of this domain gives the boundary of the instability region of the system.

The aim of this section is therefore to evaluate the convexity region in which our system is symmetric hyperbolic. This is easy because we observe that system (2) is a particular case of the one-dimensional nonlinear elasticity, and Boillat and Ruggeri have evaluated the main field [16]. In our notation we have

$$\mathbf{u}' \equiv \frac{1}{\theta}(-\pi, q, -1),$$

where θ is the dimensionless absolute temperature of a perturbed state given by [10]

$$\theta = r + 4\mathrm{e}^{-2\lambda}\lambda.$$

Therefore in this case we obtain

$$\theta Q = (\delta q)^2 + \left(\frac{\pi}{\theta} \delta\theta - \delta\pi \right) \delta d + \frac{1}{\theta} \delta\theta \delta u > 0, \qquad \forall\, (\delta d, \delta q, \delta g) \neq 0$$

that imply

$$Q^* = \left(\frac{\pi}{\theta} \delta\theta - \delta\pi \right) \delta d + \frac{1}{\theta} \delta\theta \delta u > 0, \qquad \forall\, (\delta d, \delta g) \neq 0. \tag{17}$$

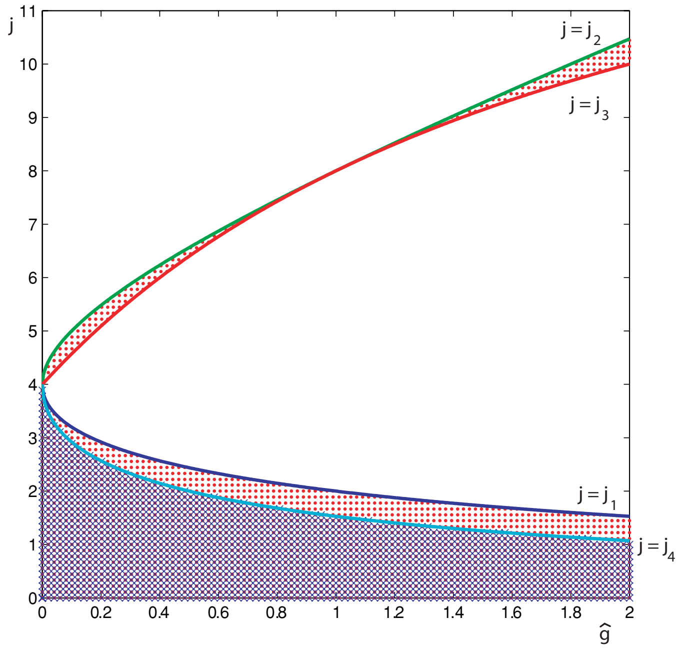

Figure 2. Hyperbolicity region (see also figure 1) and convexity domain (dark grey region) in the space state $(\hat{g}, j)$.

Simple calculations reveal that (17) is true if and only if the associated matrix of the quadratic form

$$\mathbf{Q}^* \equiv \begin{pmatrix} a_0 & b_0 \\ b_0 & c_0 \end{pmatrix} \tag{18}$$

with

$$\begin{cases} a_0 = \dfrac{\widehat{g}(j-8)^2 + (j-4)^2}{(4-j)j^2} \\ b_0 = \dfrac{(\widehat{g}(j-16) + (j-4))(j-8)}{(j-4)j^2} \\ c_0 = -\dfrac{(\widehat{g}(j-16) + 2(j-4))(-4 + \widehat{g}(j-16) + j)}{(j-4)j^2} \end{cases} \tag{19}$$

is positive definite.

It is easy to see that $a_0 > 0$ if $j < 4$, and $\det \mathbf{Q}^*$ for $j < 4$ is positive if and only if

$$j < j_4 \tag{20}$$

with

$$j_4 = 2(2 + \widehat{g} - \sqrt{\widehat{g}(4 + \widehat{g})}). \tag{21}$$

According to the general theory the convexity region $\mathcal{D}_c$ is a subset of $\mathcal{D}_h$:

$$\mathcal{D}_c : \{j < j_4\} \subset \mathcal{D}_h \tag{22}$$

and is depicted in figure 2.

4.1. Thermal equilibrium states, melting point and thermodynamic stability

Thermal equilibrium states under no external force correspond to $d = 0$, $g = 0$; then in the previous variables they can be rewritten as $j = 2$, $\hat{g} = \lambda$. By considering the intersection between the lines $j = 2$ and the curve $j = j_1$ (see figure 2), we notice the fact that the thermal equilibrium states are inside the hyperbolicity domain if $\lambda < 1$. And this fact is consistent with the result [10] that the sound velocity now is the root of (see $(10)_2$)

$$w_E^2 = 4\mathrm{e}^{-2\lambda} \frac{1 - \lambda}{2 + 7\lambda}. \tag{23}$$

On the other hand, by considering the intersection between the line $j = 2$ and the curve $j = j_4$ (see figure 2), we understand that the requirement for the equilibrium state under no external force to be in the convexity domain, that is the requirement of thermodynamic stability of the equilibrium states means $\lambda < 1/2$. Therefore the melting point with the value $\lambda = 1/2$ is the critical state in the sense that it is on the boundary of the convexity domain and therefore becomes to be thermodynamically unstable [14].

By similar reasoning, we can conclude that only the state within the convexity domain are thermodynamically stable and the states on the boundary of the convexity domain are the critical states (melting points under nonzero external forces).

5. Shock waves

We consider a shock wave propagating in a reference equilibrium state $d = g = 0$. Taking into account the well-known Rankine–Hugoniot conditions associated with system (6):

$$-\widetilde{s}[\mathbf{F}] + [\mathbf{G}] = 0$$

($\widetilde{s}$ is the shock speed, and the bracket [ ] indicates the jump of the quantify across the shock front).

In this case, introducing the dimensionless speed $s = \widetilde{s}/(a_e\Omega)$ it is easy to verify the existence of three families of shocks.

- The characteristic shock $s = 0$, which in the space of states (d, j) is represented by the curve C^0 of the equation

$$g = \tfrac{1}{3}d \tag{24}$$

  and $q = 0$.
- The sonic shocks with velocities

$$s = \pm\sqrt{\frac{2G\,\mathrm{e}^{-2\lambda}(J - G^3)}{J^2 d}} \qquad (G = \mathrm{e}^g,\ J = \mathrm{e}^d), \tag{25}$$

and curves C^+ and C^- with the equation $g(d)$ which is the implicit solution of

$$J^2(1 - 2\lambda) + G^4(1 + 4\widehat{g} + d) - GJ\{2(1 + \widehat{g}) + d\} = 0 \tag{26}$$

and $q = -sd$. An explicit expression of $g(d)$ for weak shocks was obtained in [10].

For example, for $\lambda = 1/8$ figure 3 represents the sonic shocks and the characteristic (or contact) shock. From a mathematical point of view the Rankine–Hugoniot curves also pass in the non-convexity region (right side of the curve Γ in figure 3). But it is simple matter to see that for any $\lambda < 1/2$ the admissible shock region satisfying the Lax condition is the one for which $d < 0$. Therefore the shock process $\mathcal{S}_p$ is always in the convexity region

$$\mathcal{S}_p \in \mathcal{D}_c. \tag{27}$$

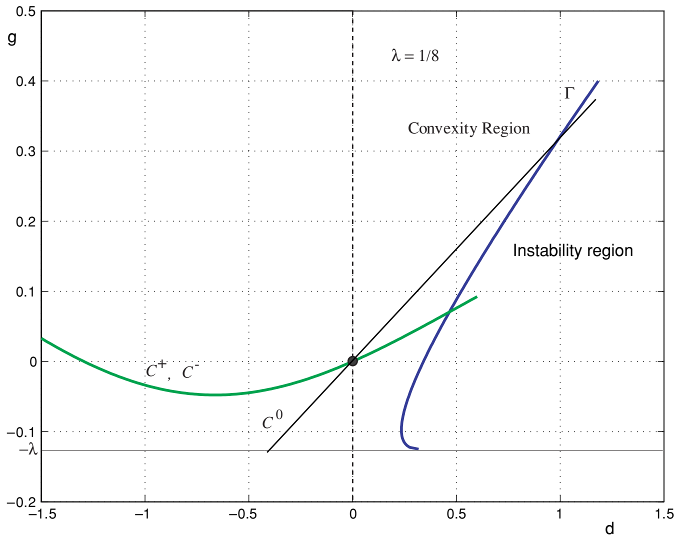

Figure 3. Rankine–Hugoniot curves for the characteristic shock C^0 and the sonic shocks C^+ and C^- in the state space (d, g) with $\lambda = 1/8$. The curve Γ is the boundary of the convexity domain.

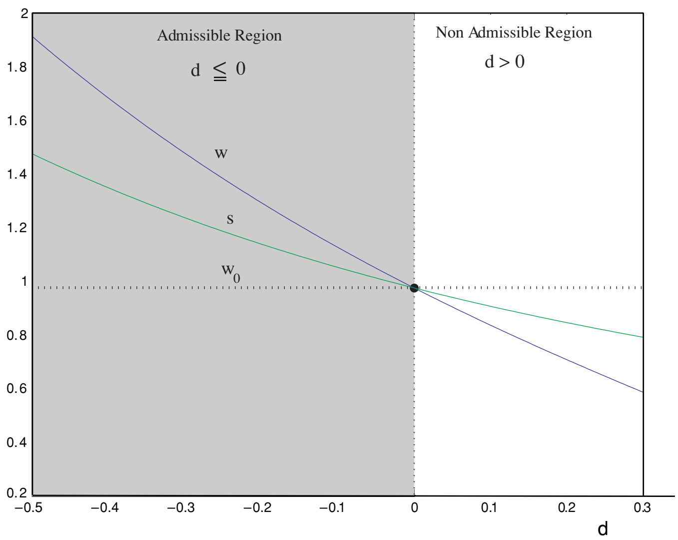

Figure 4. Admissible Lax region for shocks is shown as the grey region. The plots represent the velocities w, s and w_E normalized by the unperturbed velocity w_E versus the dimensionless deformation d.

In fact for any λ taking into account (10), (25) and (26) along $C^{\pm}$ (see (26)), we obtain

$$w_E^2 < s^2 < w^2 \tag{28}$$

if and only if $d < 0$ see figure 4.

Therefore we conclude that the admissible shocks C^+, C^- and C^0 are always processed in the convexity regions. See figure 5 for different values of λ. The Γ curves indicate, for different values of λ, the boundaries of the convexity region (the left side of Γ). We observe

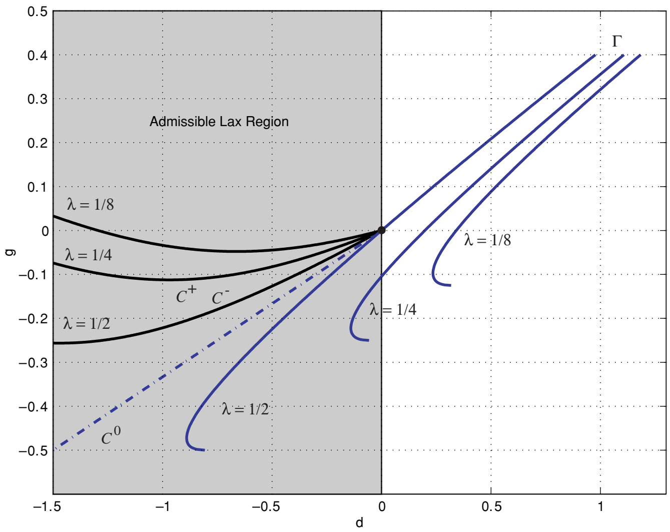

Figure 5. Rankine–Hugoniot curves for the characteristic shock C^0 and the sonic shocks C^+ and C^- in the state space (d, g) with $\lambda = 1/8$, $1/4$ and $1/2$. The curves Γ are the boundaries of the convexity region.

that for $\lambda = 1/2$ (melting point) the reference equilibrium state is on the boundary of the convexity region.

6. Conclusions

It is well known that the physics of nonlinear waves in one-dimensional anharmonic crystal lattices has a long history and has been useful to find out new concepts in the research fields of nonlinear waves and of nonlinear mechanics. Here we have clarified the differential structures of the continuum model of crystal lattices by considering both mechanical and thermodynamical properties in terms of the variables in the space of state.

In this analysis, we have found the importance of the thermal vibration, or more exactly the variance of the displacement of a constituent atom, as one of the independent variables in the model. In a thermo-elastic model, however, the temperature, or the variance of the conjugate momentum in our terminology, has usually been adopted as an independent variable. Owing to the explicit use of the thermal vibration in our model, we can analyse dynamical states of the system, especially those near the melting point.

Now let us summarize the results obtained here. First of all we have determined explicitly the differential structure of the model determining in the space of states the region in which the system is strictly hyperbolic and symmetric. The convexity region in which the system is symmetric contains the thermodynamically stable states, and its boundary corresponds to the melting points with and without external force.

Furthermore we have shown that all the admissible processes of shock type are always in the region of convexity, namely in the thermodynamically stable region.

Having the analytical results obtained here we are now being able to study, for example, the Riemann problem and the interaction between acceleration waves and shock waves, which will soon be reported.

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