Mathematical Model for Diamond-Type Crystals with Impurities or Defects

D. Opriş and I.D. Albu

Abstract

This work develops the geometry and dynamics of diamond-type crystals with impurities or defects and symmetry from the perspective of Lagrangian mechanics. We begin by formulating continuous-discret network for diamond-type crystals, then we formulate the continuous-discret Lagrange-d'Alembert principle, Noether's theorem and momentum equation for diamond-type crystals with impurities are given. Several detailed examples are given to illustrate the theory.

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Key Words: diamond-type crystal, Lagrange-d'Alembert principle, Noether theorem.

1 Introduction

The diamond-type crystals are among the most widely studied crystals in literature and the usual theories supply results in good agreement with the experiments [5]. These theories are formulated in terms of the invariants of some representations of the space group O_h^7 [2]. In [6] the case of crystals with impurities is studied and consideration of a distribution of lattice group, described by the nonintegrable distribution of lattice bases. A broad overview of the paper is as follows. We begin by describing continuous-discret network diamond-type crystal, using some representations of the space group O_h^7 [2]. The methodology from [1], is adapted for continuous-discret mechanics [3],[4], and continuous-discret Lagrange-d'Alembert principle for diamond-type crystals is given. The description of the distorted crystal structure can be realized by considering a constraint $\mathcal{S}$. The equations of motions can be written in terms of the usual Euler-Lagrange operator. Following this, we add the hypothesis of symmetry and we develop evolution equation for the momentum that generalizes the usual conservation laws associated to a symmetry group. Several detailed examples are given to ilustrate the theory.

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2 Continuous-discret network for diamond-type crystals

Let $\mathbf{Z}$ be the ring of integers and let $\mathbf{N}$ be the set of all natural numbers. The metric space $(\mathbf{D}_\infty, \delta)$, where

$$\mathbf{D}_\infty = \{n = (n_0, n_1, n_2, n_3) \in \mathbf{Z}^4 | n_0 + n_1 + n_2 + n_3 \in \{0, 1\}\} \tag{2.1}$$

and

$$\delta : \mathbf{D}_\infty \times \mathbf{D}_\infty \longrightarrow \mathbf{N}\ ,\ \delta(n, n') = \sum_{i=0}^{3} |n_i - n'_i| \tag{2.2}$$

is a discret parametric space for the ,,infinite" crystal having the structure of diamond [2]. The group of all isometries of the space $(\mathbf{D}_\infty, \delta)$ is isomorphic to the space group O_h^7 [1]. For each $n \in \mathbf{D}_\infty$ we consider the neighbours order k of n, that is the elements of the set

$$\mathcal{V}^{(k)}(n) = \{n' \in \mathbf{D}_\infty | \delta(n, n') = k\}. \tag{2.3}$$

In particular

$$\mathcal{V}^{(1)}(n) = \{n^\alpha \mid \alpha = 0, 1, 2, 3\}, \tag{2.4}$$

where

$$n^\alpha = n + \varepsilon(n) e^\alpha \qquad \varepsilon(n) = (-1)^{n_0 + n_1 + n_2 + n_3} \tag{2.5}$$

$\{e^\alpha\}$ is the canonical basis of $\mathbf{R}^4$. By considering

$$(n^\alpha)^\beta = n^{\alpha\beta} = n + \varepsilon(n) e^\alpha + \varepsilon(n^\alpha) e^\beta\ ,\ \alpha, \beta \in \{0, 1, 2, 3\}\ ,\ \alpha \neq \beta$$

$$n^{\alpha\alpha} = n\ ,\ n^{\alpha\beta} \neq n^{\beta\alpha}\ ,\ \alpha \neq \beta\ , \tag{2.6}$$

we obtain the second neighbours of n

$$\mathcal{V}^{(2)}(n) = \{n^{\alpha\beta} | \ \alpha \neq \beta\ \alpha, \beta \in \{0, 1, 2, 3\}\} \tag{2.7}$$

and the third neighbours of n

$$\mathcal{V}^{(3)}(n) = \{n^{\alpha\beta\gamma} | \alpha \neq \beta \neq \gamma\ \ \alpha, \beta, \gamma \in \{0, 1, 2, 3\}\} \tag{2.8}$$

Let $N \in \mathbf{N}$, $N > 3$, be a fixed natural number and let $\mathbf{Z}_N$ be the quotient space $\mathbf{Z}/(\mathrm{N}\mathbf{Z})$. We will obtain a parametric space for the ,,finite" crystal having the structure of diamond by using the set

$$\mathbf{D} = \{n = [n_0, n_1, n_2, n_3] \in (\mathbf{Z}_N)^4 | n_0 + n_1 + n_2 + n_3 \in \{0, 1\}\} \tag{2.9}$$

If $[a, b] \subset \mathbf{R}$ is an interval, then the set $\mathcal{R} = [a, b] \times \mathbf{D}$ will be called the *continuous-type network* for diamond-type crystals. Let $q : \mathcal{R} \longrightarrow \mathbf{R}^m$, $(m \geq 1)$, be a C^1-function (with respect to $t \in [a, b]$) and

$$q(t,n) = (q^i(t,n)) \ , \ i = \overline{1,m} \ , \ \dot{q}\ (t,n) = \frac{dq(t,n)}{dt} \ , \ (t,n) \in \mathcal{R}$$

$$q^\alpha(t,n) = q(t,n^\alpha) - q(t,n) \ , \ n^\alpha \in \mathcal{V}^{(1)}_{(n)} \ , \ q^{\alpha\beta}(t,n) = q^{\alpha\beta}(t,n^{\alpha\beta}) - q(t,n) \ ,$$

(2.10) $$n^{\alpha\beta} \in \mathcal{V}^{(2)}_{(n)}.$$

The space of functions

(2.11) $$\mathcal{L}^2(\mathcal{R}) = \{q : \mathcal{R} \longrightarrow \mathbf{R}^m | \int_a^b \sum_{n\in\mathbf{D}} \delta_{ij} q^i(t,n) q^j(t,n) < \infty\}$$

with the canonical scalar product is a Hilbert space. Let the space

(2.12) $$\Omega = \{q \in \mathcal{L}^2(\mathcal{R}) | q(a,n) = q_1(n) \ , \ q(b,n) = q_2(n) \ , \ \forall n \in \mathbf{D})\},$$

with q_1, q_2 fixed. The tangent space to Ω in $q \in \Omega$ is given by

(2.13) $$T_q(\Omega) = \{\eta : \mathcal{R} \longrightarrow \mathbf{R}^m | \eta(a,n) = 0 \ , \ \eta(b,n) = 0 \ , \ \forall \in \mathbf{D}\},$$

where

(2.14) $$\eta(t,n) = \left.\frac{dq(\varepsilon,t,n)}{d\varepsilon}\right|_{\varepsilon=0}$$

and $q(\varepsilon,t,n) \in \Omega$, $q(0,t,n) = q(t,n)$, $\varepsilon \in I \subset \mathbf{R}$, $0 \in I$. For a C^1-function $F : \Omega \longrightarrow \mathbf{R}$, the variation δF is

(2.15) $$\delta F : T_q\Omega \longrightarrow \mathbf{R} \ , \ \delta F(\eta) = \left.\frac{dF(q(\varepsilon))}{d\varepsilon}\right|_{\varepsilon=0}.$$

The element $q \in \Omega$ is called a *critical point* for F if $\delta F(\eta) = 0$, $\forall \eta \in T_q\Omega$.

3 Continuous-discret Lagrange-d'Alembert principle for diamond-type crystals

Consider the sets

(3.1) $$\begin{aligned} &\Omega^1 = \{q^\alpha(t,n) \ , \ q \in \Omega \ , \ \alpha \in \{0,1,2,3\} \ , \ (t,n) \in \mathcal{R}\} \\ &\Omega^2 = \{q^{\alpha\beta}(t,n) \ , \ q \in \Omega \ , \ \alpha \neq \beta \ \alpha,\beta \in \{0,1,2,3\} \ , \ (t,n) \in \mathcal{R}\} \\ &\overset{\bullet}{\Omega} = \{\dot{q}\ (t,n) \ , \ q \in \Omega \ , \ (t,n) \in \mathcal{R}\} \end{aligned}$$

and the C^1-function $L : \mathcal{R} \times \Omega \times \Omega^1 \times \Omega^2 \times \overset{\bullet}{\Omega} \longrightarrow \mathbf{R}$, given by

(3.2) $$L(t,n) = L(t,n,q(t,n),q^\alpha(t,n),q^{\alpha\beta}(t,n),\dot{q}\ (t,n)) \ , \ (t,n) \in \mathcal{R}.$$

The functional

(3.3)
$$\mathcal{A}(q) = \int_a^b \sum_{n\in\mathbf{D}} L(t,n)dt$$

is called the *action* of L with respect to $q \in \Omega$.

Theorem 3.1 [4] **(First variation formula)**. The variation $\delta\mathcal{A}(q)$ of the action $\mathcal{A}(q)$ is

(3.4)
$$\delta\mathcal{A}(q)(\eta) = \int_a^b \sum_{n\in\mathbf{D}} E_i(\overline{L})\eta^i(t,n)dt \ , \ \eta \in T_q\Omega,$$

where

(3.5)
$$E_i(\overline{L}) = \frac{d\overline{L}(t,n)}{dq^i(t,n)} - \frac{d}{dt}(\frac{\partial\overline{L}(t,n)}{\partial\dot{q}^i(t,n)})$$

(3.6)
$$\overline{L}(t,n) = L(t,n) + \sum_{\alpha=0}^{3} L(t,n^\alpha) + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3} L(t,n^{\alpha\beta}).$$

From theorem 3.1 we deduce

Theorem 3.2 (Discret continuous variation principle). An element $q \in \Omega$ is a critical point for $\mathcal{A}(q)$ if and only if

(3.7)
$$\frac{d\overline{L}(t,n)}{dq^i(t,n)} - \frac{d}{dt}\left(\frac{\partial\overline{L}(t,n)}{\partial\dot{q}^i(t,n)}\right) = 0 \ , \ \forall(t,n)\in\mathcal{R} \ , \ i=\overline{1,m}.$$

Example. The Lagrange function of the atoms of the crystal with respect to their equilibrum positions is given by [2],[5]

(3.8)
$$\begin{aligned} L(t,n) &= \frac{1}{2}m\delta_{ij}\dot{q}^i(t,n)\dot{q}^j(t,n) - \frac{1}{2}\sum_{\alpha=0}^{3}\phi_{ij\alpha}q^{i\alpha}(t,n)q^{j\alpha}(t,n) - \\ &- \frac{1}{2}\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\phi_{ij\alpha\beta}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n) \ , \ (t,n)\in\mathcal{R} \ , \ i,j=1,2,3, \end{aligned}$$

where

$$\phi_{ij\alpha} = \phi_{ji\alpha} = \text{const} \ , \ \phi_{ij\alpha\beta} = \phi_{ji\alpha\beta} = \text{const}.$$

From (3.7) we obtain

(3.9)
$$m\delta_{ij}\frac{d^2q^i(t,n)}{dt^2} = \sum_{\alpha=0}^{3}\phi_{ij\alpha}q^{j\alpha}(t,n) + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\phi_{ij\alpha\beta}q^{j\alpha\beta}(t,n) \ , \ \forall(t,n)\in\mathcal{R}.$$

The system of equations (3.9) corresponds to the system of equations used in lattice dynamics of diamond-type crystals (the model of Born-von Karman).

For the study of the dynamics in crystals it is useful to introduce some so-called motions of order α and $\alpha\beta$. Let $f^a : \mathcal{R} \times \Omega \times \Omega^1 \times \Omega^2 \times \dot{\Omega} \longrightarrow \mathbf{R}$, $a = \overline{1,p}$, be a C^1-function with respect to $t \in [a,b]$, $q \in \Omega$, $q^\alpha \in \Omega^1$, $q^{\alpha\beta} \in \Omega^2$, $\dot{q} \in \dot{\Omega}$. We put

$$f^a(t,n) = f^a(t,n,q(t,n),\ q^\alpha(t,n),\ q^{\alpha\beta}(t,n),\ \dot{q}^i\ (t,n))\ ,\ (t,n) \in \mathcal{R} \tag{3.10}$$

and suppose that

$$\text{rang} \left\| \frac{\partial f^a(t,n)}{\partial q^{\alpha i}(t,n)} \right\| = p < m\ ,\ \alpha = 0,1,2,3; \tag{3.11}$$

$$\text{rang} \left\| \frac{\partial f^a(t,n)}{\partial q^{\alpha\beta i}(t,n)} \right\| = p < m\ ,\ \alpha,\beta = 0,1,2,3\ ,\ \alpha \neq \beta; \tag{3.12}$$

$$\text{rang} \left\| \frac{\partial f^a(t,n)}{\partial \dot{q}^i(t,n)} \right\| = p < m. \tag{3.13}$$

Let us consider the set

(3.14)

$$\mathcal{S} = \{(q(t,n), q^\alpha(t,n), q^{\alpha\beta}(t,n), \dot{q}\ (t,n)) \in \Omega \times \Omega^1 \times \Omega^2 \times \dot{\Omega}\ | f^a(t,n) = 0\ ,\ a = \overline{1,p}\}$$

For a generic element $q \in \Omega$, for $\mathcal{S}$, let $\eta \in T_q\Omega$ be the tangent vector to Ω satisfying the conditions

$$\frac{\partial f^a(t,n)}{\partial q^{\alpha i}(t,n)} \eta^i(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ \alpha \in \{0,1,2,3\},\ \text{fixed.} \tag{3.15}$$

η is called the *virtual variation of the order* α for the system $(\Omega, L, \mathcal{S})$, where L is given by (3.2) and $\mathcal{S}$ is given by (3.14).

The Lagrange-d'Alembert principle of order α is the following: an admissible element $q \in \Omega$ is called a motion of the order α for the system $(\Omega, L, \mathcal{S})$ if $[E]_i(\overline{L})\eta^i(t,n) = 0\ ,\ \forall (t,n) \in \mathcal{R}$, for all virtual variations of the order α.

Proposition 3.3. The motion of the order α is given by

$$E_i(\overline{L})(t,n) = \mu_a^\alpha \frac{\partial f^a(t,n)}{\partial q^{i\alpha}(t,n)}\ \ i = \overline{1,m}, \tag{3.16}$$

$$f^a(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ \alpha \text{ fixed}\ ,\ (t,n) \in \mathcal{R}.$$

The elements $\eta \in T_q\Omega$ satisfying the conditions

$$\frac{\partial f^a(t,n)}{\partial q^{\alpha\beta i}(t,n)} \eta^i(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ \alpha \neq \beta\ ,\text{fixed} \tag{3.17}$$

are called the *virtual variations of the order* $\alpha\beta$ for the system $(\Omega, L, \mathcal{S})$.

The Lagrange-d'Alembert principle of order $\alpha\beta$ is the following: an admissible element $q \in \Omega$ is called a motion of the order $\alpha\beta$ for the system $(\Omega, L, \mathcal{S})$ if $[E]_i(\overline{L})\eta^i(t,n) = 0\ ,\ \forall (t,n) \in \mathcal{R}$, for all virtual variations of the order $\alpha\beta$.

Proposition 3.4. The motion of the order $\alpha\beta$ is given by

$$E_i(\overline{L})(t,n) = \mu_a^{\alpha\beta} \frac{\partial f^a(t,n)}{\partial q^{i\alpha\beta}(t,n)} \ , i = \overline{1,m}, \tag{3.18}$$

$$f^a(t,n) = 0 \ , \ a = \overline{1,p} \ , \ \alpha, \beta \text{ fixed} \ , \ (t,n) \in \mathcal{R}.$$

The elements $\eta \in T_q\Omega$ satisfying the conditions

$$\frac{\partial f^a(t,n)}{\partial \dot{q}^i(t,n)} \eta^i(t,n) = 0 \ , \ a = \overline{1,p}, \tag{3.19}$$

are called the *virtual variations* for $(\Omega, L, \mathcal{S})$.

The Lagrange-d'Alembert principle is: an admissible element $q \in \Omega$ is called a *motion* for the system $(\Omega, L, \mathcal{S})$ if $[E]_i(\overline{L})\eta^i(t,n) = 0 \ , \ \forall (t,n) \in \mathcal{R}$, for all virtual variations.

Proposition 3.5 [3]. The motion is given by

$$E_i(\overline{L}(t,n) = \mu_a \frac{\partial f^a(t,n)}{\partial \dot{q}^i(t,n)}) \ , \ i = \overline{1,m}, \tag{3.20}$$

$$f^a(t,n) = 0 \ , \ a = \overline{1,p} \quad , (t,n) \in \mathcal{R}.$$

4 Constraint distribution on the space $\Omega \times \Omega^1 \times \Omega^2 \times \overset{\bullet}{\Omega}$

The description of the distorted crystal structure can be realised by considering a constraint $\mathcal{S}$ given by (3.14). If we choose the affine constraints of the form

$$f^a(t,n) = q^{a\alpha}(t,n) + A_r^{a\alpha} q^{r\alpha}(t,n) - \gamma^{a\alpha}(t,n), \tag{4.1}$$

where

$$A_r^{a\alpha}(t,n) = A_r^{a\alpha}(q(t,n)) \ , \ \gamma^{a\alpha}(t,n) = \gamma^{a\alpha}(q(t,n)), \tag{4.2}$$

$a = \overline{1,p} \ , \ r = \overline{p+1,m} \ , \ \alpha \in \{0,1,2,3\}$, fixed, then from the Lagrange-d'Alembert principle of order α we get.

Proposition 4.1. The motion of the order α is given by

$$E_r(\overline{L}) = A_r^{a\alpha}(t,n) E_a(\overline{L}) \qquad a = \overline{1,p} \ , \ r = \overline{p+1,m}, \tag{4.3}$$

$$q^{a\alpha}(t,n) + A_r^{a\alpha}(t,n) q^{r\alpha}(t,n) - \gamma^{a\alpha}(t,n) = 0 \ , \ (t,n) \in \mathcal{R}.$$

Now we define the constrained Lagrangian of order α, L_c, by substituting the constraints (4.2) into the Lagrangian (3.2).

$$L_C(t,n) = L(t,n,q(t,n), \ -A_r^{a\alpha}(t,n)q^{r\alpha}(t,n) + \gamma^{a\alpha}(t,n), \ q^{r\alpha}(t,n),$$

$$q^\beta(t,n), \ q^{\gamma\beta}(t,n), \ \dot{q}\ (t,n)) \tag{4.4}$$

Theorem 4.2. The equations of the motion of order α are

$$
\begin{aligned}
E_r(\overline{L_C}) \quad &- \quad A_r^{a\alpha}(t,n)E_a^{\alpha}(\overline{L_C}) = \left[A_r^{a\alpha}(t,n^{\alpha}) - A_r^{a\alpha}(t,n)\right]\frac{\partial L(t,n^{\alpha})}{\partial q^{a\alpha}(t,n)}+ \\
&+ \quad B_{rs}^{a\alpha}(t,n)q^{s\alpha}(t,n)\frac{\partial L(t,n)}{\partial q^{a\alpha}(t,n)} + \gamma_r^{a\alpha}(t,n)\frac{\partial L(t,n)}{\partial q^{a\alpha}(t,n)}
\end{aligned} \tag{4.5}
$$

$$q^{a\alpha}(t,n) + A_r^{a\alpha}(t,n)q^{r\alpha}(t,n) - \gamma^{a\alpha}(t,n) = 0 \ , \ a = \overline{1,p} \ , \ r,s = \overline{p+1,m},$$

where

$$B_{rs}^{a\alpha}(t,n) = A_r^{b\alpha}(t,n)\frac{\partial A_s^{a\alpha}(t,n)}{\partial q^b(t,n)} - \frac{\partial A_s^{a\alpha}(t,n)}{\partial q^r(t,n)}, \tag{4.6}$$

$$\gamma_r^{a\alpha}(t,n) = \frac{\partial \gamma^{a\alpha}(t,n)}{\partial q^r(t,n)} - A_r^{b\alpha}(t,n)\frac{\partial \gamma^{a\alpha}(t,n)}{\partial q^b(t,n)}, \tag{4.7}$$

$$
\begin{aligned}
E_a^{\alpha}(\overline{L_C}) \quad &= \quad \frac{\partial L_C(t,n)}{\partial q^a(t,n)} - \sum_{\substack{\beta = 0 \\ \beta \neq \alpha}}^{3} \frac{\partial (L_C(t,n) + L_C(t,n^{\beta}))}{\partial q^{a\beta}(t,n)} - \\
&- \quad \sum_{\substack{\beta,\gamma = 0 \\ \beta \neq \gamma}}^{3} \frac{\partial (L_C(t,n) + L_C(t,n^{\beta\alpha}))}{\partial q^{a\beta\gamma}(t,n)} - \frac{d}{dt}\left(\frac{\partial L_C(t,n)}{\partial \dot{q}^{a}(t,n)}\right)
\end{aligned} \tag{4.8}
$$

Let the affine constraints of the form

$$f^a(t,n) = q^{a\alpha\beta}(t,n) + A_r^{a\alpha\beta}(t,n)q^{r\alpha\beta}(t,n) - \gamma^{a\alpha\beta}(t,n), \tag{4.9}$$

where

$$
\begin{aligned}
&A_r^{a\alpha\beta}(t,n) = A_r^{a\alpha\beta}(q(t,u)) \ , \ \gamma^{a\alpha\beta}(t,n) = \gamma^{a\alpha\beta}(q(t,n)) \\
&a = \overline{1,p} \ , \ r = \overline{p+1,m} \ , \ \alpha,\beta \in \{0,1,2,3\} \ , \ \alpha \neq \beta \text{ fixed}
\end{aligned} \tag{4.10}
$$

From the Lagrange-d'Alembert principle of order $\alpha\beta$ we obtain
Proposition 4.3. The motion of the order $\alpha\beta$ is given by

$$E_r(\overline{L}) = A_r^{a\alpha\beta}(t,n)E_a(\overline{L}) \ \ a = \overline{1,p} \ , \ r = \overline{p+1,m}, \tag{4.11}$$

$$q^{a\alpha\beta}(t,n) + A_r^{a\alpha\beta}(t,n)q^{r\alpha\beta}(t,n) - \gamma^{a\alpha\beta}(t,n) = 0 \ , \ (t,n) \in \mathcal{R}. \tag{4.12}$$

Define the constrained Lagrangian of order $\alpha\beta$, L_C, by substituting the constraints (4.12) into the Lagrangian (3.2):

$$
\begin{aligned}
L_C(t,n) \quad &= \quad L(t,n,q(t,n),q^{\gamma}(t,n),-A_r^{a\alpha\beta}(t,n)q^{r\alpha\beta}(t,n)+ \\
&+ \quad \gamma^{a\alpha\beta}(t,n),q^{r\alpha\beta}(t,n),q^{\gamma\delta}(t,n),\dot{q}\,(t,n)).
\end{aligned} \tag{4.13}
$$

Theorem 4.4. *The equations of the motion of order* $\alpha\beta$ *are*

$$E_r(\overline{L_C}) - A_r^{a\alpha\beta}(t,n)E_a^{\alpha\beta}(\overline{L_C}) = \left[A_r^{a\alpha\beta}(t,n^{\alpha\beta}) - A_r^{a\alpha\beta}(t,n)\right]\frac{\partial L(t,n^{\alpha\beta})}{\partial q^{a\alpha\beta}(t,n)} +$$

$$(4.13)' \qquad + B_{rs}^{a\alpha\beta}(t,n)q^{s\alpha\beta}(t,n)\frac{\partial L(t,n)}{\partial q^{a\alpha\beta}(t,n)} + \gamma_r^{a\alpha\beta}(t,n)\frac{\partial L(t,n)}{\partial q^{a\alpha\beta}(t,n)},$$

$$q^{a\alpha\beta}(t,n) + A_r^{a\alpha\beta}(t,n)q^{r\alpha\beta}(t,n) - \gamma_r^{a\alpha\beta}(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ r,s = \overline{p+1,m},$$

where

$$(4.14) \qquad B_{rs}^{a\alpha\beta}(t,n) = A_r^{a\alpha\beta}(t,n)\frac{\partial A_s^{a\alpha\beta}(t,n)}{\partial q^b(t,n)} - \frac{\partial A_s^{a\alpha\beta}(t,n)}{\partial q^r(t,n)},$$

$$(4.15) \qquad \gamma_r^{a\alpha\beta}(t,n) = \frac{\partial \gamma^{a\alpha\beta}(t,n)}{\partial q^r(t,n)} - A_r^{b\alpha\beta}(t,n)\frac{\partial \partial^{a\alpha\beta}(t,n)}{\partial q^b(t,n)},$$

$$(4.16) \qquad \begin{aligned} E_a^{\alpha\beta}(\overline{L_C}) &= \frac{\partial L_C(t,n)}{\partial q^a(t,n)} - \sum_{\gamma=0}^{3}\frac{\partial(L_C(t,n) + L_C(t,n^\gamma))}{\partial q^{a\gamma}(t,n)} - \\ &- \sum_{\substack{\gamma,\,\delta=0 \\ \gamma\neq\delta,\,\gamma\neq\alpha,\beta}}^{3}\frac{\partial(L_C(t,n) + L_C(t,n^{\gamma\delta}))}{\partial q^{a\gamma\delta}(t,n)} - \frac{d}{dt}\left(\frac{\partial L_C(t,n)}{\partial \dot{q}^a(t,n)}\right). \end{aligned}$$

Finally let us consider affine constraints of the form

$$(4.17) \qquad f^a(t,n) = \dot{q}^a(t,n) + A_r^a(t,n)\dot{q}^r(t,n) - \gamma^a(t,n)\ \ a = \overline{1,p}\ ,\ r = \overline{p+1,m},$$

where

$$(4.18) \qquad A_r^a(t,n) = A_r^a(q(t,n))\ ,\ \gamma^a(t,n) = \gamma^a(q(t,n)).$$

From the Lagrange-d'Alembert principle we obtain
Propositin 4.5. The motion is given by

$$(4.19) \qquad E_r(\overline{L}) = A_r^a(t,n)E_a(\overline{L}),$$

$$(4.20) \qquad \dot{q}^a(t,n) + A_r^a(t,n)\dot{q}^r(t,n) - \gamma^a(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ r = \overline{r+1,m}.$$

Let now the constrained Lagrangian L_C obtained by substituting the constraints (4.20) in the Lagrangian

$$(4.21) \qquad L(t,n) = L(n, q(t,n), q^\alpha(t,n), q^{\alpha\beta}(t,n), \dot{q}\ (t,n)),$$

that is
(4.22)

$$L_C(t,n) = L(n, q(t,n), q^\alpha(t,n), q^{\alpha\beta}(t,n), -A_r^a(t,n)\dot{q}^r(t,n) + \gamma^a(t,n), \dot{q}^r(t,n)).$$

Theorem 4.6. *The equations of the motion are*

$$(4.23)\quad E_r(\overline{L_C}) - A^a_r(t,n)\frac{d\overline{L_C}(t,n)}{dq^s(t,n)} = B^a_{rs}(t,n)\frac{\partial L(t,n)}{\partial \dot{q}^a(t,n)}\dot{q}^s(t,n) + \frac{\partial L(t,n)}{\partial \dot{q}^a(t,n)}\gamma^a_r(t,n),$$

$$\dot{q}^a(t,n) + A^a_r(t,n)\dot{q}^r(t,n) - \gamma^a(t,n) = 0\ ,\ a = \overline{1,p}\ ,\ r,s = \overline{p+1,m},$$

where

$$(4.24)\qquad B^a_{rs}(t,n) = \frac{\partial A^a_r(t,n)}{\partial q^r(t,n)} - \frac{\partial A^a_s(t,n)}{\partial q^r(t,n)} + A^b_r(t,n)\frac{\partial A^a_s(t,n)}{\partial q^b(t,n)} - A^b_s\frac{\partial A^a_r(t,n)}{\partial q^b(t,n)},$$

$$(4.25)\qquad \gamma^a_r(t,n) = \frac{\partial \gamma^a(t,n)}{\partial q^r(t,n)} - A^b_r(t,n)\frac{\partial \gamma^a(t,n)}{\partial q^b(t,n)} + \gamma^b(t,n)\frac{\partial A^a_r(t,n)}{\partial q^b(t,n)}.$$

Examples. 1) Let the Lagrangian

$$L(t,n) = \frac{1}{2}\delta_{ij}\dot{q}^i(t,n)\dot{q}^j(t,n) - \frac{1}{4}\sum_{\alpha=0}^{3}\delta_{ij}q^{i\alpha}(t,n)q^{j\alpha}(t,n) -$$

$$(4.26)\qquad -\frac{1}{4}\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\delta_{ij}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n)$$

and the constraints $q^{30}(t,n) - q^2(t,n)q^{10}(t,n) = 0$.

We have

$$L_C(t,n) = \frac{1}{2}\delta_{ij}\dot{q}^i(t,n)\dot{q}^j(t,n) - \frac{1}{4}(1+q^2(t,n)^2)q^{10}(t,n)^2 - \frac{1}{4}q^{20}(t,n)^2 -$$

$$-\frac{1}{4}\sum_{\alpha=1}^{3}\delta_{ij}q^{i\alpha}(t,n)q^{j\alpha}(t,n) - \frac{1}{4}\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\delta_{ij}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n)$$

and the equations of the motion of order „0" are given by

$$\ddot{q}^1(t,n) + q^2(t,n)\ddot{q}^3(t,n) = \left(1 + \frac{1}{2}q^2(t,n)^2 + \frac{1}{2}q^2(t,n^0)^2\right)q^{10}(t,n) +$$

$$+\sum_{\alpha=1}^{3}(q^{1\alpha}(t,n) + q^2(t,n)q^{3\alpha}(t,n)) + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}(q^{1\alpha\beta}(t,n) + q^2(t,n)q^{3\alpha\beta}(t,n)),$$

$$\ddot{q}^2(t,n) = \sum_{\alpha=0}^{3}q^{2\alpha}(t,n) + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}q^{2\alpha\beta}(t,n) - \frac{1}{2}q^2(t,n)q^{10}(t,n)^2,$$

$$q^{30}(t,n) = q^2(t,n)q^{10}(t,n)\ .$$

2) Let the Lagrangian given by (4.26) and the constraint

$$q^{312}(t,n)-q^{2}(t,n)q^{112}(t,n)=0.$$

We have

$$L_C(t,n)=\frac{1}{2}\delta_{ij}\dot{q}^{i}(t,n)\dot{q}^{j}(t,n)-\frac{1}{4}\sum_{\alpha=0}^{3}\delta_{ij}q^{i\alpha}(t,n)q^{j\alpha}(t,n)-$$

$$-\frac{1}{4}(1+q^{2}(t,n)^{2})q^{112}(t,n)^{2}-\frac{1}{4}q^{212}(t,n)^{2}-\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq1,\,\beta\neq2}}^{3}\delta_{ij}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n)$$

and the equations of the motions of order „12" are the followings

$$\ddot{q}^{1}(t,n)+q^{2}(t,n)\ddot{q}^{3}(t,n)=(1+\frac{1}{2}q^{2}(t,n)^{2}+\frac{1}{2}q^{2}(t,n^{12})^{2})q^{112}(t,n)+$$

$$+\sum_{\alpha=0}^{3}(q^{1\alpha}(t,n)+q^{2}(t,n)q^{3\alpha}(t,n))+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq1,\,\beta\neq2}}^{3}(q^{1\alpha\beta}(t,n)+q^{2}(t,n)q^{3\alpha\beta}(t,n)),$$

$$\ddot{q}^{2}(t,n)=\sum_{\alpha=0}^{3}q^{2\alpha}(t,n)+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq1,\,\beta\neq2}}^{3}q^{2\alpha\beta}(t,n)-\frac{1}{2}q^{2}(t,n)q^{112}(t,n)^{2},$$

$$q^{312}(t,n)=q^{2}(t,n)q^{112}(t,n).$$

Consider the Lagrangian (4.26) and the constraint

$$\dot{q}^{3}(t,n)-q^{2}(t,n)\dot{q}^{1}(t,n)=0.$$

We have

$$L_C(t,n)=\frac{1}{2}(1+q^{2}(t,n)^{2})\dot{q}^{1}(t,n)^{2}+\frac{1}{2}\dot{q}^{2}(t,n)^{2}-\frac{1}{4}\sum_{\alpha=0}^{3}\delta_{ij}q^{i\alpha}(t,n)q^{j\alpha}(t,n)-$$

$$-\frac{1}{4}\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\delta_{ij}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n)$$

and the equations of the motiom are given by

$$(1+q^{2}(t,n))\ddot{q}^{1}(t,n)+\dot{q}^{2}(t,n)\ddot{q}^{3}(t,n)=-2q^{2}(t,n)\dot{q}^{1}(t,n)\dot{q}^{2}(t,n)-$$

$$-\sum_{\alpha=0}^{3}(q^{1\alpha}(t,n)+q^{2}(t,n)q^{3\alpha}(t,n))-\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}(q^{1\alpha\beta}(t,n)+q^{2}(t,n)q^{3\alpha\beta}(t,n))$$

$$\ddot{q}^{2}(t,n)=q^{2}(t,n)\dot{q}^{1}(t,n)^{2}+\sum_{\alpha=0}^{3}q^{2\alpha}(t,n)+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}q^{2\alpha\beta}(t,n)\ .$$

5 Noether's Theorem for diamond-type crystals

Let G be a Lie group acting (at the left) on Ω by $(g,q) \in G \times \Omega \longrightarrow gq = \overline{q}$, $(gq)(t,n) = \overline{q}(t,n,g)$. Let $\mathcal{G}$ be the Lie algebra of G and $\mathcal{G}^*$ the linear dual af $\mathcal{G}$. To each vector $\xi \in \mathcal{G}$ corresponds an one-parameter subgroup of G, $\exp(\varepsilon\xi)$, $\varepsilon \in I \subset \mathbf{R}$, whose action on Ω determines

$$(5.1) \qquad \xi_\Omega(t,n) = \frac{d}{d\varepsilon}[\exp(\varepsilon\xi)q(t,n)]_{\varepsilon=0} \ , \ \forall (t,n) \in \mathcal{R}.$$

From (5.1), we obtain

$$(5.2) \qquad \xi^i_\Omega(t,n) = K^i_a(t,n)\xi^a \ , \ i = \overline{1,m} \ , \ a = \overline{1,r} \ , \ r = \dim G,$$

where

$$(5.3) \qquad \xi = \xi^a e_a \in \mathcal{G} \ , \ K^i_a = \left. \frac{d\overline{q}^i(t,n,\exp(\varepsilon e_a))}{d\varepsilon} \right|_{\varepsilon=0} .$$

Let $\overline{q}^p$ be the canonical prolongation of the action of G on $\Omega \times \Omega^1 \times \Omega^2 \times \overset{\bullet}{\Omega}$. The Lie group G is called a symmetry group of the system (Ω, L), where L is autonomous in t, if

$$(5.4) \qquad L \circ \overline{q}^p(t,n,g) = L(t,n) \ , \ \forall (t,n) \in \mathcal{R} \ , \ \forall g \in G.$$

The corresponding α-momentum map is the function $\mathcal{J}_\alpha : \Omega \times T_q\Omega^1 \longrightarrow \mathcal{G}^*$, given by

$$(5.5) \qquad \mathcal{J}_\alpha(t,n) = \frac{\partial L(t,n)}{\partial q^{i\alpha}(t,n)} K^i_a(t,n^\alpha)e^a \ , \ \alpha \in \{0,1,2,3\} \ \text{,fixed.}$$

The corresponding $\alpha\beta$-momentum map is the function $\mathcal{J}_{\alpha\beta} : \Omega \times T_q\Omega^2 \longrightarrow \mathcal{G}^*$,

$$(5.6) \qquad \mathcal{J}_{\alpha\beta}(t,n) = \frac{\partial L(t,n)}{\partial q^{i\alpha\beta}(t,n)} K^i_a(t,n^{\alpha\beta})e^a \ , \ \alpha,\beta \in \{0,1,2,3\} \ , \ \alpha \neq \beta \ \text{,fixed.}$$

The corresponding continuous momentum map is $\mathcal{J} : \Omega \times T_q \overset{\bullet}{\Omega} \longrightarrow \mathcal{G}^*$,

$$(5.7) \qquad \mathcal{J}(t,n) = \frac{\partial L(t,n)}{\partial \dot{q}^i(t,n)} K^i_a(t,n)e^a.$$

Theorem 5.1. (Noether's Theorem for diamond-type crystals). For each solution of the Euler-Lagrange equations (3.7),

$$(5.8) \qquad \sum_{\alpha=0}^{3} \mathcal{J}^\alpha_\alpha(t,n) + \sum_{\substack{\alpha,\beta=0 \\ \alpha\neq\beta}}^{3} \mathcal{J}^{\alpha\beta}_{\alpha\beta}(t,n) + \frac{d\mathcal{J}(t,n)}{dt} = 0,$$

where

$$\mathcal{J}^{\alpha}_{\alpha}(t,n)=\mathcal{J}_{\alpha}(t,n^{\alpha})-\mathcal{J}_{\alpha}(t,n)\ ,\mathcal{J}^{\alpha\beta}_{\alpha\beta}(t,n)=\mathcal{J}_{\alpha\beta}(t,n^{\alpha\beta})-\mathcal{J}_{\alpha\beta}(t,n).$$

Suppose that the Lagrangian L does not depends on q^j , j fixed. Locally the system (Ω,L) admits a symmetry group G_j. The action on Ω is given by

$$\overline{q}^i(t,n)=q^i(t,n)\ ,\ \overline{q}^j(t,n)=q^j(t,n)+\alpha^j\ ,\ i\neq j,\ \alpha^j\in\mathbf{R}. \tag{5.9}$$

We have $K^j_i(t,n)=\delta^i_j$ and from (5.6) we obtain

$$\sum_{\alpha=0}^{3}\frac{\partial(L(t,n)+L(t,n^{\alpha}))}{\partial q^{j\alpha}(t,n)}+\sum_{\substack{\alpha\ ,\ \beta\ =\ 0\\ \alpha\neq\beta}}^{3}\frac{\partial(L(t,n)+L(t,n^{\alpha\beta}))}{\partial q^{j\alpha\beta}(t,n)}-\frac{d}{dt}\left(\frac{\partial L(t,n)}{\partial\dot{q}^j(t,n)}\right)=0. \tag{5.10}$$

The coordinate q^i is called a *cyclic coordinate.*

6 Momentum equation for diamond-type crystals with impurities

In this sections we shall use the Lagrange-d'Alembert principle to derive an equation for a generalized momentum as a consequence of the symmetries. We assume that the action of G on Ω is free and proper. The orbit through a point $q\in\Omega$ is denoted by Orb$(q)=\{gq|g\in G\}$. Let $\mathcal{S}\subset\Omega\times\Omega^1\times\Omega^2\times\overset{\bullet}{\Omega}$ and $T_q\mathcal{S}$ the virtual variation. If $S_q=T_q\mathcal{S}\cap T_q(\text{orb}(\overline{q}^p))\neq\{0\}$, where $\overline{q}^p$ is the canonical prolongation of the action of G on $\Omega\times\Omega^1\times\Omega^2\times\overset{\bullet}{\Omega}$ then let $\mathcal{G}(q)=\{\xi\in\mathcal{G}|\xi_{\Omega}(q)\in S_q\}$.

The α-nonholomic momentum map $\mathcal{J}_{\alpha}$ is defined by

$$\mathcal{J}_{\alpha}(t,n)=\frac{\partial L(t,n)}{\partial q^{i\alpha}(t,n)}\xi^i(t,n^{\alpha}),\ (t,n)\in\mathcal{R}, \tag{6.1}$$

where

$$\xi^i(t,n^{\alpha})=K^i_a(t,n^{\alpha})\xi^a(t,n^{\alpha})\ ,\ \xi(t,n^{\alpha})=\xi(q(t,n^{\alpha})),\ \alpha\in\{0,1,2,3\}\ ,\ \alpha\text{ fixed.}$$

The $\alpha\beta$-nonholonomic momentum map $\mathcal{J}_{\alpha\beta}$ is defined by

$$\mathcal{J}_{\alpha\beta}(t,n)=\frac{\partial L(t,n)}{\partial q^{i\alpha\beta}(t,n)}\xi^i(t,n^{\alpha\beta})\ ,\ (t,n)\in\mathcal{R}, \tag{6.2}$$

where

$$\xi^i(t,n^{\alpha\beta})=K^i_a(t,n^{\alpha\beta})\xi^a(t,n^{\alpha\beta}),\ \alpha\ ,\beta\in\{0,1,2,3\}\ ,\ \alpha\neq\beta\ ,\text{fixed.}$$

The continuous nonholonomic momentum map $\mathcal{J}$ is defined by

$$\mathcal{J}(t,n)=\frac{\partial L(t,n)}{\partial\dot{q}^i(t,n)}\xi^i(t,n)\qquad,(t,n)\in\mathcal{R}, \tag{6.3}$$

where

$$\xi^i(t,n) = K^i_a(t,n)\xi^a(t,n).$$

Theorem 6.1. Assume that the Lagrangian L is invariant under the group action and $\xi(q) \in \mathcal{G}(q)$. Then any solution of the Lagrange-d'Alembert equation for a $\mathcal{S}$ satisfies the following momentum equation

$$\sum_{\alpha=0}^{3} \mathcal{J}^{\alpha}_{\alpha}(t,n) + \sum_{\alpha,\beta=0}^{3} \mathcal{J}^{\alpha\beta}_{\alpha\beta}(t,n) + \frac{d\mathcal{J}(t,n)}{dt} = \sum_{\alpha=0}^{3} \frac{\partial L(t,n)}{\partial q^{i\alpha}(t,n)} K^i_a(t,n)\xi^{a\alpha}(t,n) +$$

$$(6.4) \qquad + \sum_{\substack{\alpha,\,\beta\,=\,0\\ \alpha\,\neq\,\beta}}^{3} \frac{\partial L(t,n)}{\partial q^{i\alpha\beta}(t,n)} K^i_a(t,n)\xi^{a\alpha\beta}(t,n) + \frac{\partial L(t,n)}{\partial \dot{q}(t,n)} K^i_a(t,n)\frac{d\xi^a(t,n)}{dt}.$$

At a fixed point $q_0 \in \Omega$, we consider a basis $\{e_1,\dots e_p, e_{p+1},\dots e_r\}$ of $\mathcal{G}$ such that the first p elements form a basis of $\mathcal{G}(q_0)$. Thus $r = \dim\mathcal{G}$, $p = \dim\mathcal{G}(q_0)$, which, by assumption, is locally constant. We can introduce a similar basis $\{e_1(q),\dots e_p(q), e_{p+1}(q),\dots,e_r(q)\}$ for $q \in \Omega$. Let a change of basis matrix

$$(6.5) \qquad e_u(q(t,n)) = e_u(t,n) = \Psi^v_u(q(t,n))e_v(q_0(t,n)) = \Psi^v_u(t,n)e_v \ , \ u,v = \overline{1,r}.$$

Here the matrix (Ψ^b_a) is an $r \times r$ invertible matrix. By the definitions (5.5), (5.6), (5.7) we can write

$$\mathcal{J}_{\alpha a}(t,n) = \frac{\partial L(t,n)}{\partial q^{i\alpha}(t,n)}[e_a(t,n^{\alpha})]^i_{\Omega},$$

$$(6.6) \qquad \mathcal{J}_{\alpha\beta a}(t,n) = \frac{\partial L(t,n)}{\partial q^{i\alpha\beta}(t,n)}[e_a(t,n^{\alpha\beta})]^i_{\Omega},$$

$$\mathcal{J}_{a}(t,n) = \frac{\partial L(t,n)}{\partial \dot{q}^{i}(t,n)}[e_a(t,n)]^i_{\Omega} \ , a = \overline{1,p} \ , \ (t,n) \in \mathcal{R},$$

where

$$[e_a(t,n^{\alpha})]^i_{\Omega} = K^i_a(t,n^{\alpha}), \ [e_a(t,n^{\alpha\beta})]^i_{\Omega} = K^i_a(t,n^{\alpha\beta}) \ , \ [e_a(t,n)]^i_{\Omega} = K^i_a(t,n).$$

Theorem 6.2. The momentum equation in a moving basis $\{e_n(t,n)\}_{u=\overline{1,r}}$ is given by

$$\sum_{\alpha=0}^{3} \mathcal{J}^{\alpha}_{\alpha a}(t,n) + \sum_{\substack{\alpha,\,\beta\,=\,0\\ \alpha\,\neq\,\beta}}^{3} \mathcal{J}^{\alpha\beta}_{\alpha\beta a} + \frac{d\mathcal{J}_a(t,n)}{dt} = \sum_{\alpha=0}^{3} \Lambda^b_a(t,n,n^{\alpha})\mathcal{J}_{\alpha b}(t,n) +$$

$$+ \sum_{\substack{\alpha,\,\beta\,=\,0\\ \alpha\,\neq\,\beta}}^{3} \Theta^b_a(t,n,n^{\alpha})\mathcal{J}_{\alpha\beta b}(t,n) + \Gamma^b_a(t,n)\mathcal{J}_b(t,n) + \sum_{\alpha=0}^{3} \frac{\partial L(t,n)}{\partial q^{i\alpha}(t,n)} \Lambda^s_b(t,n,n^{\alpha})[e_s(t,n^{\alpha})]^i_{\Omega} +$$

$$+ \sum_{\substack{\alpha,\,\beta\,=\,0\\ \alpha\,\neq\,\beta}}^{3} \frac{\partial L(t,n)}{\partial q^{i\alpha\beta}(t,n)} \Theta^s_b(t,n,n^{\alpha\beta})[e_s(t,n^{\alpha\beta})]^i_{\Omega} +$$

$$+\frac{\partial L(t,n)}{\partial \dot{q}^i(t,n)}\Gamma^s_{bj}(t,n)\dot{q}^j(t,n)[e_s(t,n)]^i_\Omega \; a=\overline{1,p} \; s=\overline{p+1,r}, \tag{6.7}$$

where

$$\begin{aligned} \Lambda^v_a(t,n,n^\alpha) &= \Psi^{\alpha u}_a(t,n)\tilde{\Psi}^v_u(t,n^\alpha), \\ \Theta^v_a(t,n,n^\alpha) &= \Psi^{\alpha\beta u}_a(t,n)\tilde{\Psi}^v_u(t,n^{\alpha\beta}), \\ \Gamma^v_{aj}(t,n) &= \frac{\partial \Psi^u_a(t,n)}{\partial q^j(t,n)}\tilde{\Psi}^v_u(t,n)\;, a=\overline{1,p}\;,\; v=\overline{1,r}. \end{aligned} \tag{6.8}$$

Examples. 1) Let the Lagrangian

$$\begin{aligned} L(t,n) &= \frac{1}{2}\delta_{ij}\dot{q}^i(t,n)\dot{q}^j(t,n) - \frac{1}{4}\sum_{\alpha=0}^{3}\delta_{ij}q^{i\alpha}(t,n)q^{j\alpha}(t,n) - \\ &- \frac{1}{4}\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\delta_{ij}q^{i\alpha\beta}(t,n)q^{j\alpha\beta}(t,n) \end{aligned} \tag{6.9}$$

and the constraint

$$q^{30}(t,n) - q^2(t,n)q^{10}(t,n) = 0. \tag{6.10}$$

The constraint and the Lagrangian are invariants under the $\mathbf{R}^2$-action on $\mathbf{R}^3$ given by

$$(q^1,q^2,q^3) \longrightarrow (q^1+\lambda, q^2, q^3+\mu).$$

The tangent spaces to the orbits of this action are given by

$$T_{q(t,n)}(\mathrm{Orb}(q(t,n))) = \mathrm{span}\{(1,0,0),(0,0,1)\}$$

and the virtual vectors of the constraints are given by

$$S_{q(t,n)} = \mathrm{span}\{(1,0,q^2(t,n)),(0,1,0)\}.$$

It follows

$$T_{q(t,n)}(\mathrm{Orb}(q(t,n))) \cap S_{q(t,n)} = \mathrm{span}\{1,0,q^2(t,n)\}$$

and

$$\xi^{q(t,n)}_\Omega = (1,0,q^2(t,n)) \;\;, \xi^{q(t,n)} = (1,q^2(t,n)).$$

The nonholonomic momentum maps in this case are

$$\begin{aligned} \mathcal{J}_\alpha(t,n) &= -\tfrac{1}{2}q^{1\alpha}(t,n) - \tfrac{1}{2}q^{3\alpha}(t,n)q^2(t,n^\alpha), \\ \mathcal{J}_{\alpha\beta}(t,n) &= -\tfrac{1}{2}q^{1\alpha\beta}(t,n) - \tfrac{1}{2}q^{3\alpha\beta}(t,n)q^2(t,n^{\alpha\beta}), \\ \mathcal{J}(t,n) &= \dot{q}^1(t,n) + \dot{q}^3(t,n)q^2(t,n). \end{aligned}$$

The momentum equation is given by

$$\sum_{\alpha=0}^{3} q^{1\alpha}(t,n)+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}(q^{1\alpha\beta}(t,n)+q^{3\alpha\beta}(t,n)q^{2}(t,n^{\alpha\beta}))+\sum_{\alpha=1}^{3} q^{3\alpha}(t,n)q^{2}(t,n^{\alpha})+$$

$$+q^{2}(t,n)q^{2}(t,n^{0})q^{10}(t,n)+\ddot{q}^{1}(t,n)+\ddot{q}^{3}(t,n)q^{2}(t,n)=0.$$

2) Let the Lagrangian (6.9) and the constraint

$$q^{312}(t,n)-q^{2}(t,n)q^{112}(t,n)=0.$$

The momentum equation is given by

$$\sum_{\alpha=0}^{3} q^{1\alpha}(t,n)+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq 1,\,\beta\neq 2}}^{3} q^{1\alpha\beta}(t,n)+\sum_{\alpha=0}^{3} q^{3\alpha}(t,n)q^{2}(t,n^{\alpha})+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq 1,\,\beta\neq 2}}^{3} q^{3\alpha\beta}(t,n)q^{2}(t,n^{\alpha\beta})+$$

$$+(1+q^{2}(t,n)q^{2}(t,n^{12}))q^{112}(t,n)+\ddot{q}^{1}(t,n)+\ddot{q}^{3}(t,n)q^{2}(t,n)=0.$$

3) Let the Lagrangian (6.9) and the constraint

$$\dot{q}^{3}(t,n)-q^{2}(t,n)\dot{q}^{1}(t,n)=0.$$

The momentum equation is given by

$$\sum_{\alpha=0}^{3}(q^{1\alpha}(t,n)+q^{3\alpha}(t,n)q^{2}(t,n^{\alpha}))+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}(q^{1\alpha\beta}(t,n)+q^{3\alpha\beta}(t,n)q^{2}(t,n^{\alpha\beta}))+$$

$$+(1+q^{2}(t,n)^{2})\ddot{q}^{1}(t,n)+q^{2}(t,n)\dot{q}^{2}(t,n)\dot{q}^{1}(t,n)=0.$$

4) For the same Lagrangian and the constraints

$$\dot{q}^{3}(t,n)-q^{2}(t,n)\dot{q}^{1}(t,n)=0,$$
$$q^{30}(t,n)-q^{2}(t,n)q^{10}(t,n)=0,$$
$$q^{312}(t,n)-q^{2}(t,n)q^{312}(t,n)=0,$$

the momentum equation is

$$(1+q^{2}(t,n)^{2})\ddot{q}^{1}(t,n)+q^{2}(t,n)\dot{q}^{1}(t,n)\dot{q}^{2}(t,n)+(1+q^{2}(t,n^{0})^{2})q^{2}(t,n)q^{10}(t,n)+$$

$$+(1+q^{2}(t,n^{12}))q^{112}(t,n)+\sum_{\alpha=0}^{3}(q^{1\alpha}(t,n)+q^{3\alpha}q^{2}(t,n^{\alpha}))+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta,\,\alpha\neq 1,\,\beta\neq 2}}^{3}(q^{1\alpha\beta}+q^{3\alpha\beta}q^{2}(t,n^{\alpha\beta}))=0.$$

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References

[1] A.M.Bloch, P.S.Krishnaprasad, J.E.Marsden, R.M.Murray, *Nonholonomic mechanical system with symmetry*, Archive for Rational Mechanics and Analysis, C.D.S. Tehnical Report 90-013 California Institute of Technology, (1995).

[2] N.Cotfas, *A mathematical model for diamond-type crystals*, J. Phys. A. Math. Gen 28(1995), 1371-1379.

[3] D.Crăciun and D.Opriş, *Discrete-continuous dynamical systems with symmetry*, Balkan Journal of Geometry and Its Applications, 2,2 (1997), 35–49.

[4] D.Opriş and I. Albu, *On the discrete-continuous dynamical systems*, Analalele Universităţii ,,Al.I.Cuza", Iaşi (1995).

[5] C.Patel, W.F.Sherman and G.R.Wilkinsen, *J. Phis. C. Solid State Phis.* 17(1984), 6063-69.

[6] A.Trzesowski, *Gauge theory of dislocations*, International Journal of Theoretical Physics vol. 26, 11(1987).

West University of Timişoara
Department of Mathematics
B-dul V.Pârvan 4
1900 Timişoara, Romania