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A HAMILTONIAN APPROACH TO THE DISCRETE-CONTINUOUS DYNAMICAL SYSTEMS IN DIAMOND-TYPE CRYSTALS

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Abstract

In a previous paper [5] we formulated a discrete-continuous Lagrangean formalism for the dynamical systems in crystals. In this Note we propose in the same context the Hamiltonian aspect.

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1 Introduction.

An important aspect in the study of the dynamics in crystals is the space modifications of the atoms of crystals with respect to their equilibrium positions. Such dynamics may appear during the phenomena of growth or of fusion of crystals. The space modification take place either in all directions or in privileged directions. The crystalline particles can be influenced at different levels in the neighbourhood of a centre of crystallization. In the mathematical model the influence between two neighbouring atoms is expressed by differences or some difference combinations, like in the model Born-von Karmann (in our considerations this role is played by the functions S). Our study refers only to the neighbours of order 1 and 2 (where there exist sensible influences).

The interest of the Hamiltonian point of view derives from the expression of the Hamilton equations as a differential system of order 1, wich permits some posibilities of study. Also the Hamilton equations may appear directly from Lagrangeans in certain conditions of non-degeneration.

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2 The Parametric Space for diamond-type cristals

The metric space $(\mathbf{D}_\infty, \delta)$, where

$$\mathbf{D}_\infty = \{n = (n^0, n^1, n^2, n^3) \in \mathbf{Z}^4 | n^0 + n^1 + n^2 + n^3 \in \{0, 1\}\}$$

and

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

is a discrete parametric space for the „infinite" crystal having the structure of diamond. The group of all isometries of the space $(\mathbf{D}_\infty, \delta)$ is isomorphic to the space group O_h^7 (see [2]). This group is the group generated by the transformations Λ ,$\Lambda_\sigma : \mathbf{D}_\infty \longrightarrow \mathbf{D}_\infty$,

$$\Lambda(n^0, n^1, n^2, n^3) = (-n^0 + 1, -n^1, -n^2, -n^3) \ ,$$
$$\Lambda_\sigma(n^0, n^1, n^2, n^3) = (n^{\sigma(0)}, n^{\sigma(1)}, n^{\sigma(2)}, n^{\sigma(3)}) \ ,$$

where $\sigma \in \sum_4$. For each $n \in \mathbf{D}_\infty$ we consider the neighbours of order k of n, that is the elements of the set

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

In particular,

$$\mathcal{V}^{(1)} = \{n_\alpha | \alpha = 0, 1, 2, 3\} \ ,$$

where $n_\alpha = n + \varepsilon(n) e_\alpha \ , \ \varepsilon(n) = (-1)^{n^0+n^1+n^2+n^3}$.
($\{e_\alpha\}$ is the canonical base of $\mathbf{R}^4$) are the first neighbours of n; by considering,

$$\begin{array}{l} (n_\alpha)_\beta = n_{\alpha\beta} = n + \varepsilon(n) e_\alpha + \varepsilon(n_\alpha) e_\beta \ , \\ n_{\alpha\alpha} = n \ , \ n_{\alpha\beta} \neq n_{\beta\alpha} \ , \ \alpha \neq \beta \end{array} \quad \alpha, \beta \in \{0, 1, 2, 3\} \ , \ \alpha \neq \beta \ ,$$

we obtain the second neighbours of n:

$$\mathcal{V}^{(2)} = \{n_{\alpha\beta} | \alpha \neq \beta \ , \ \alpha, \beta\{0, 1, 2, 3\}\} \ .$$

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

$$D = \{n = [n^0, n^1, n^2, n^3] \in (\mathbf{Z}_N)^4 | n^0 + n^1 + n^2 + n^3 \in \{0, 1\}\} \ .$$

If $[a, b] \subset \mathbf{R}$ is an interval, then the set $\mathcal{R} = [a, b] \times D$ is called the continuous-discrete network for diamond-type crystals. For a C^1-function (with respect to the first variable) $q : \mathcal{R} \longrightarrow \mathbf{R}^m$ we denote $q(n) = q(t, n)$, respectively $(q^i(n)) = (q^i(t, n))$, $(\dot{q}^i(n)) = (\dot{q}^i(t, n))$.

3 The Euler-Lagrange Equations. A non-linear Connection

Let $T\mathbf{R}^m$ be the tangent bundle of $\mathbf{R}^m$ and $S : \mathbf{R}^m \times \mathbf{R}^m \longrightarrow \mathbf{R}^p$, $T : \mathbf{R}^m \times \mathbf{R}^m \longrightarrow \mathbf{R}^q$ functions of class C^∞. We denote $S_\alpha = S(x, x(\alpha))$, $\alpha = 0,1,2,3$, $T_{\alpha\beta} = S(x, x(\alpha\beta))$, $\alpha, \beta \in \{0,1,2,3\}$, $\alpha \neq \beta$, x, $x(\alpha)$, $x(\alpha\beta) \in \mathbf{R}^m$. For $n \in D$, let $q(n) \in \mathbf{R}^m$, $\dot{q}\ (n) \in \mathbf{R}^m$, the position and the velocity associated to n and $q(n_\alpha), q(n_{\alpha\beta}) \in \mathbf{R}^m$ the position associated to n_α, $n_{\alpha\beta}$. We obtain, for $n \in D$, the elements of $T\mathbf{R}^m \times \mathbf{R}^p \times \mathbf{R}^q$, $(q(n), \dot{q}\ (n), S(q(n), q(n_\alpha)), T(q(n), q(n_{\alpha\beta})))$.

Let $L : T\mathbf{R}^m \times \mathbf{R}^p \times \mathbf{R}^q \longrightarrow \mathbf{R}$, $L = L(x, v, S_\alpha, T_{\alpha\beta})$ be a C^∞-function and we denote $L(n) = L(q(n), \dot{q}\ (n), S_\alpha(q(n), q(n_\alpha)), T_{\alpha\beta}(q(n), q(n_{\alpha\beta})))$.

The functional

$$\mathcal{A}(q) = \int_{t_0}^{t_1} \sum_{n \in D} L(n) dt$$

is called the action of L with respect to q.

For $(q(n), \dot{q}\ (n)) \in T\mathbf{R}^m$ let $(\lambda, \dot{\lambda}) : T\mathbf{R}^m \times (-a, a) \longrightarrow T\mathbf{R}^m$ denote by $\lambda(q(n), \varepsilon) = q(n, \varepsilon)$, $\dot{\lambda}\ (q(n), \varepsilon) = \dot{q}\ (n, \varepsilon)$ with $q(n, 0) = q(n)$, $\dot{q}\ (n, 0) = \dot{q}$ (n) and we put

$$\eta(n) = \left. \frac{\partial q(n,\varepsilon)}{\partial \varepsilon} \right|_{\varepsilon=0} ; \ \dot{\eta}\ (n) = \left. \frac{\partial\ \dot{q}\ (n,\varepsilon)}{\partial \varepsilon} \right|_{\varepsilon=0} .$$

The first variation of the function $\mathcal{A}$ with respect to λ is:

$$\delta\mathcal{A} = \int_{t_0}^{t_1} \sum_{\substack{m \in D \\ \delta(m,n) > 2}} A(t,m) dt + \int_{t_0}^{t_1} A(t,n) dt + \int_{t_0}^{t_1} \sum_{\alpha=0}^{3} A(t, n_\alpha) dt +$$
$$\int_{t_0}^{t_1} \sum_{\substack{\alpha,\beta=0 \\ \alpha\neq\beta}}^{3} A(t, n_{\alpha\beta}) dt ,$$

where:

$$A(t,n) = \frac{\partial L}{\partial x^i}(n)\eta^i(n) + \sum_{\alpha=0}^{3} \frac{\partial L}{\partial S^a_\alpha}(n) \frac{\partial S^a_\alpha}{\partial x^i}(n)\eta^i(n) +$$
$$\sum_{\substack{\alpha,\beta=0 \\ \alpha\neq\beta}}^{3} \frac{\partial L}{\partial T^b_{\alpha\beta}}(n) \frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n)\eta^i(n) + + \sum_{\alpha=0}^{3} \frac{\partial L}{\partial S^a_\alpha}(n) \frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n)\eta^i(n_\alpha) +$$

$$\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3} \frac{\partial L}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n)\eta^i(n_{\alpha\beta}) - \frac{\partial L}{\partial v^i}(n)\dot{\eta}^i(n) .$$

From (1) we obtain

Proposition 1. The first variation of the function $\mathcal{A}$ with respect to λ is:

$$(1) \qquad \delta\mathcal{A}(q)(\eta) = \int_{t_0}^{t_1} \sum_{n\in D} e_i(L,n)\eta^i(n) + \sum_{n\in D}\frac{\partial L}{\partial v^i}(n)\eta^i(n)\Big|_{t_0}^{t_1} ,$$

where

$$(2) \qquad e_i(L,n) = \frac{\partial L}{\partial x^i}(n) + \sum_{\alpha=0}^{3}\left[\frac{\partial L}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n) + \frac{\partial L}{\partial S^a_\alpha}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n_\alpha)\right] +$$

$$+ \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\left[\frac{\partial L}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n) + \frac{\partial L}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}\right] - \frac{d}{dt}\left(\frac{\partial L}{\partial v^i}\right)(n) .$$

For $S^i_\alpha = q^i(n_\alpha) - q^i(n)$ and $T^i_{\alpha\beta}(n) = q^i(n_{\alpha\beta}) - q^i(n)$, we obtain

$$e_i(L,n) = \frac{\partial L}{\partial x^i}(n) - \sum_{\alpha=0}^{3}\left(\frac{\partial L}{\partial S^i_\alpha}(n) + \frac{\partial L}{\partial S^i_\alpha}(n_\alpha)\right) -$$

$$- \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\left(\frac{\partial L}{\partial T^i_{\alpha\beta}}(n) + \frac{\partial L}{\partial T^i_{\alpha\beta}}(n_{\alpha\beta})\right) - \frac{d}{dt}\left(\frac{\partial L}{\partial v^i}(n)\right) ,$$

given in [5].

If one imposes the standard conditions

$$q(t_0,n) = q(t_1,n) = 0 , \ \forall\, n\in D$$

then the Euler-Lagrange equations are

$$(3) \qquad e_i(L,n) = 0 , \ i = \overline{1,m} , \ n\in D .$$

For $L(n) = \frac{1}{2}m\delta_{ij}\dot{q}^i(n)\dot{q}^j(n) - \sum_{\alpha=0}^{3}\Phi_{ij\alpha}S^i_\alpha(n)S^j_\alpha(n) - \sum_{\alpha\neq\beta}\Phi_{ij\alpha\beta}T^i_{\alpha\beta}(n)T^j_{\alpha\beta}(n)$

we obtain the equations from the model Born-von Karmann.

The corresponding equations (3) are

$$g_{ij}\frac{\partial^2 q^j}{\partial t^t} = L_i + \sum_{\alpha=0}^{3} L_{i\alpha} + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3} L_{i\alpha\beta} \ ,$$

where

$$g_{ij} = \frac{\partial^2 L}{\partial v^i \partial v^j}(n) \ , \ L_i = \frac{\partial L}{\partial x^i}(n) - \dot{q}^j(n)\frac{\partial^2 L}{\partial x^j \partial v^i}(n) \ ,$$

$$L_{i\alpha} = \frac{\partial L}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n) + \frac{\partial L}{\partial S^a_\alpha}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n_\alpha) \ ,$$

$$L_{i\alpha\beta} = \frac{\partial L}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n) + \frac{\partial L}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta}) \ .$$

If $q(n), q(n_\alpha), \dot{q}\ (n_{\alpha\beta}) \in Q$ and $S : Q \times Q \longrightarrow B$, $T : Q \times Q \longrightarrow C$, where Q, B, C are differentiable manifolds and det $\left\| \frac{\partial^2 L}{\partial v^i \partial v^j}(n) \right\| \neq 0$, $\forall\, n \in D$, then, as in [3], we can prove.

Proposition 2. There exists a non-linear connection associated to the equation (3), which is uniquely determinated by L. The coefficients of this non-linear connection are:

$$N^i_j(n) = \frac{\partial G^i}{\partial v^j} + \sum_{\alpha=0}^{3} \frac{\partial G^i_\alpha}{\partial v^j} + \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3} \frac{\partial G^i_{\alpha\beta}}{\partial v^j} \tag{4}$$

where $G^i = g^{ik} L_k$, $G^i_\alpha = g^{ik} L_{k\alpha}$, $G^i_{\alpha\beta} = g^{ik} L_{k\alpha\beta}$.

4 The Hamilton Equations

Let $T^*\mathbf{R}^m$ be the cotangent bundle of $\mathbf{R}^m$ and $S : \mathbf{R}^m \times \mathbf{R}^m \longrightarrow \mathbf{R}^p$, $T : \mathbf{R}^m \times \mathbf{R}^m \longrightarrow \mathbf{R}^q$ functions of class C^∞ like in Section 3. For $n \in D$ let $q(n) \in \mathbf{R}^m$, $\dot{q}\ (n) \in \mathbf{R}^m$, $p(n) \in \mathbf{R}^m$ be the position, the velocity and the impulse associated to n [$p(n) = p(t,n)$, $(p_i(n)) = (p_i(t,n))$, $(\dot{p}_i(n)) = (\dot{p}_i(t,n))$] and $q(n_\alpha)$, $q(n_{\alpha\beta}) \in \mathbf{R}^m$, $p(n_\alpha)$, $p(n_{\alpha\beta}) \in \mathbf{R}^m$ the same elements associated to $n_\alpha, n_{\alpha\beta}$. We obtain, for $n \in D$, the elements ob $T^*\mathbf{R}^m \times \mathbf{R}^p \times \mathbf{R}^q$ of the form $(q(n), p(n), S_\alpha(q(n), q(n_\alpha)), T_{\alpha\beta}(q(n), q(n_{\alpha\beta})))$.

Let $H : T^*\mathbf{R}^m \times \mathbf{R}^p \times \mathbf{R}^q \longrightarrow \mathbf{R}$, $H = H(x, p, S_\alpha, T_{\alpha\beta})$ be a C^∞-function and we denote $H(n) = H(q(n), p(n), S_\alpha(q(n), q(n_\alpha)), T_{\alpha\beta}(q(n), q(n_{\alpha\beta})))$.

The functional

$$\mathcal{H}(q,p)=\int_{t_0}^{t_1}\sum_{n\in D}(p_i(n)\dot{q}^i(n)-H(n))dt$$

is called the action of H with respect to (p,q).

Proposition 3. The Hamilton equations for H are the followings:

$$\dot{q}^i(n)=\frac{\partial H}{\partial p_i}(n)\ ,$$

$$(5)\qquad \dot{p}_i(n)=-\left[\frac{\partial H}{\partial x^i}(n)+\sum_{\alpha=0}^{3}\left[\frac{\partial H}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n)+\frac{\partial H}{\partial S^a_\alpha}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n_\alpha)\right]+\right.$$

$$\left.+\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\left[\frac{\partial H}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n)+\frac{\partial H}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta})\right]\right]$$

Proposition 3 results by annuling the first variation of $\mathcal{H},\delta\mathcal{H}$

Remark. If $S^i_\alpha(n)=q^i(n_\alpha)-q^i(n)$, $T^i_{\alpha\beta}=q^i(n_{\alpha\beta})-q^i(n)$ then

$$\dot{p}_i(t,n)=$$

$$-\frac{\partial H}{\partial q^i}(n)-\sum_{\alpha=0}^{3}\left[\frac{\partial H}{\partial S^i_\alpha}(n)+\frac{\partial H}{\partial S^i_\alpha}(n_\alpha)\right]-\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\left[\frac{\partial H}{\partial T^i_{\alpha\beta}}(n)+\frac{\partial H}{\partial T^i_{\alpha\beta}}(n_{\alpha\beta})\right]\ .$$

Example. For L given in the model Born-von Karmann, we put

$$p_i(n)=\frac{\partial L}{\partial q^i}(n)=m\delta_{ij}\dot{q}^j(n)\ \text{ and}$$

$$H(n)=\frac{1}{2}m\delta^{ij}p_i(n)p_j(n)-\sum_{\alpha=0}^{3}\Phi_{ij\alpha}S^i_\alpha(n)S^j_\alpha(n)-\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\Phi_{ij\alpha\beta}T^i_{\alpha\beta}(n)T^j_{\alpha\beta}(n)\ .$$

The Hamilton equations in this case are:

$$\dot{q}^i(n)=\frac{1}{m}\delta^{ij}p_j(n)\ ,$$

$$\dot{p}^i(n)=-\sum_{\alpha=0}^{3}\Phi_{ij\alpha}S^j_\alpha(n)-\sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3}\Phi_{ij\alpha\beta}S^j_{\alpha\beta}(n)\ .$$

Now let $\gamma \in \{0,1,2,3\}$ be fixed, $p_\gamma \in (\mathbf{R}^p)^*$ and $H_\gamma : T\mathbf{R}^m \times (\mathbf{R}^p)^* \times \mathbf{R}^q \longrightarrow \mathbf{R}$, $H_\gamma = H(x, v, p_\gamma, S_\alpha, T_{\alpha\beta})$, $\alpha, \beta \neq \gamma$, a C^∞-function. We denote $H_\gamma(n) = H(q(n), \dot{q}\ (n), p_\gamma(n), S_\alpha(q(n), q(n_\alpha)), T_{\alpha\beta}(q(n), q(n_{\alpha\beta})))$. The action of H_γ with respect to (q, p_γ) is

$$\mathcal{H}_\gamma(q,p_\gamma) = \int_{t_0}^{t_1} \sum_{n\in D} [p_\gamma(n) S_\gamma(q(n), q(n_\gamma)) - H_\gamma(n)] dt \,.$$

Proposition 4. The Hamilton equations for H_γ are the followings:

$$S^a_\gamma(q(n), q(n_\gamma)) = \frac{\partial H_\gamma}{\partial p_{\gamma a}}(n) \,;$$

$$p_{\gamma a}(n)\frac{\partial S^a_\gamma}{\partial x^i}(n) + \sum_{\substack{\alpha=0\\ \alpha\neq\gamma}}^{3} p_{\gamma a}(n_\alpha)\frac{\partial S^a_\gamma}{\partial x^i_\alpha}(n_\alpha) = \frac{\partial H_\gamma}{\partial x^i}(n) - \frac{d}{dt}\left(\frac{\partial H_\gamma}{\partial v^i}(n)\right) +$$
$$+ \sum_{\substack{\alpha=0\\ \alpha\neq\gamma}}^{3} \left[\frac{\partial H_\gamma}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n) + \frac{\partial H_\gamma}{\partial S^a_\alpha}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n_\alpha)\right] +$$
$$+ \sum_{\substack{\alpha,\beta=0\\ \alpha\neq\beta}}^{3} \left[\frac{\partial H_\gamma}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n) + \frac{\partial H_\gamma}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta})\right]$$

By analogy, let $\gamma, \delta \in \{0,1,2,3\}$, $\gamma \neq \delta$, fixed, $p_{\gamma\delta} \in (\mathbf{R}^q)^*$ and $H_{\gamma\delta} : T\mathbf{R}^m \times \mathbf{R}^p \times (\mathbf{R}^q)^* \longrightarrow \mathbf{R}$, $H_{\gamma\delta} = H(x, v, S_\alpha, p_{\gamma\delta}, T_{\alpha\beta})$, $\alpha \neq \gamma$, $\beta \neq \delta$. We denote $H_{\gamma\delta}(n) = H(q(n), \dot{q}\ (n), S_\alpha(n), p_{\gamma\delta}(n), T_{\alpha\beta}(n))$, where $S_\alpha(n) = S_\alpha(q(n), q(n_\alpha))$, $T_{\alpha\beta}(n) = T_{\alpha\beta}(q(n), q(n_{\alpha\beta}))$, $\alpha \neq \gamma$, $\beta \neq \delta$.

The action of $H_{\gamma\delta}$ with respect to $(q, p_{\gamma\delta})$ is

$$\mathcal{H}_{\gamma\delta}(q,p_{\gamma\delta}) = \int_{t_0}^{t_1} \sum_{n\in D} [p_{\gamma\delta b}(n) T^b_{\gamma\delta}(q(n), q(n_{\gamma\delta})) - H_{\gamma\delta}(n)] dt$$

Proposition 5. The Hamilton equations for $H_{\gamma\delta}$ are the followings:

$$T^b_{\gamma\delta}(q(n), q(n_{\gamma\delta})) = \frac{\partial H_{\gamma\delta}}{\partial p_{\gamma\delta}}(n) \,;$$

$$(7) \qquad p_{\gamma\delta a}(n)\frac{\partial T^a_{\gamma\delta}}{\partial x^i}(n) + \sum_{\substack{\alpha,\beta=0,\alpha\neq\beta\\ ,\alpha\neq\gamma,\beta\neq\delta}}^{3} p_{\gamma\delta a}(n_{\alpha\beta})\frac{\partial T^a_{\gamma\delta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta}) = \frac{\partial H_{\gamma\delta}}{\partial x^i}(n) -$$

$$-\frac{d}{dt}\left(\frac{\partial H_{\gamma\delta}}{\partial v^i}(n)\right)+\sum_{\alpha=0}^{3}\left[\frac{\partial H_{\gamma\delta}}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n)+\frac{\partial H_{\gamma\delta}}{\partial S^\alpha_a}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^i_\alpha}(n_\alpha)\right]+$$
$$+\sum_{\substack{\alpha,\beta=0,\alpha\neq\beta\\ ,\alpha\neq\gamma,\beta\neq\delta}}^{3}\left[\frac{\partial H_{\gamma\delta}}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i}(n)+\frac{\partial H_{\gamma\delta}}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta})\right]$$

We can obtain Hamilton equations by considering some combinations involving the Hamiltonian function but it is necessary to impose certain conditions of non-degeneration.

Let $\overline{H}: T^*\mathbf{R}^m \times (\mathbf{R}^p)^* \times \mathbf{R}^q \longrightarrow \mathbf{R}$, $\overline{H}=\overline{H}(x,p,p_\gamma,S_\alpha,T_{\alpha\beta})$, $\alpha\neq\gamma$ be a C^∞-function. The action of $\overline{H}$ is

$$\overline{\mathcal{H}}(q,p,p_\gamma)=\int_{t_0}^{t_1}\sum_{n\in D}[p_i(n)\dot{q}^i(n)+p_{\gamma a}(n)S^a_\gamma(q(n),q(n_\gamma))-\overline{H}(n)]dt\ .$$

Proposition 6. The Hamilton equations for $\overline{H}$ is the followings:

$$\dot{q}^i(n)=\frac{\partial H}{\partial p_i}(n)\ ;$$

(8)
$$\dot{p}_i(n)+p_{\gamma a}(n)\frac{\partial S^a_\gamma}{\partial x^i}(n)+\sum_{\substack{\alpha=0,\\ ,\alpha\neq\gamma}}^{3}p_{\gamma a}(n_\alpha)\frac{\partial S^a_\gamma}{\partial x^i_\alpha}(n_\alpha)=\frac{\partial\overline{H}}{\partial x^i}(n)+$$
$$+\sum_{\substack{\alpha=0,\\ \alpha\neq\gamma}}^{3}\left[\frac{\partial\overline{H}}{\partial S^a_\alpha}(n)\frac{\partial S^a_\alpha}{\partial x^i}(n)+\frac{\partial\overline{H}}{\partial S^a_\alpha}(n_\alpha)\frac{\partial S^a_\alpha}{\partial x^a_\alpha}(n_\alpha)\right]+$$
$$+\sum_{\substack{\alpha,\beta=0,\\ \alpha\neq\gamma}}^{3}\left[\frac{\partial\overline{H}}{\partial T^b_{\alpha\beta}}(n)\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n)+\frac{\partial\overline{H}}{\partial T^b_{\alpha\beta}}(n_{\alpha\beta})\frac{\partial T^b_{\alpha\beta}}{\partial x^i_{\alpha\beta}}(n_{\alpha\beta})\right]\ .$$

Example. For the Lagrangean L given in [6],

$$L(n)=\frac{1}{2}m\delta_{ij}\dot{q}^i(n)\dot{q}^j(n)-\frac{1}{2}\Phi_{ij0}S^i_0(n)S^j_0(n)-\Phi_{ij03}T^i_{03}(n)T^j_{03}(n)$$

we put

$$\frac{\partial L}{\partial v^i}(n)=\frac{1}{m}\delta_{ij}\dot{q}^j(n)=p_i(n)\ ,\ \frac{\partial L}{\partial S^i_0}(n)=\Phi_{ij0}S^j_0(n)=p_{0i}(n)$$

and we obtain the following Hamilton equations:

$$\dot{q}\,(n) = \frac{1}{m}\delta^{ij}p_j(n)\ ;$$
$$S_0^i(n) = -\Phi_0^{ij}p_{0j}(n)\ ,$$
$$\dot{p}_i(n) + p_{0i}(n^0) - p_{0i}(n) = (\Phi_{ij03} + \Phi_{ji03})[T_{03}^j(n) + T_{03}^j(n^0)]\ ,$$

where (Φ_{ij0}) is non-degenerated, but (Φ_{ij03}) may be degenerated.

Using basic ideas from algebraic geometry the authors of [1] consider a class of discrete mechanical systems as the cellular automata on finite lattices. The idea is to construct an algebraic analog for the configuration space and the Lagrangean as well for the phase space and the symplectic structure on it. Also, the algebraic functions substitute the usual differential calculus.

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