

## AN ALGEBRAIC, ENERGY CONSERVING FORMULATION OF CLASSICAL MOLECULAR AND NEWTONIAN $n$ -BODY INTERACTION

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Communicated by Fred Brauer, August 14, 1972

**1. Introduction.** In this note we will develop a unifying theory of collisionless  $n$ -body problems which includes both Newtonian and classical molecular forces. By using only *differences* to simulate physical concepts and *difference* equations to determine dynamical behavior, the resulting theory will be completely arithmetic in nature. Thus, we will have the advantages of mathematical simplicity and computer compatibility. The formulation will have special value for problems involving large amounts of energy, since it will be energy conserving.

**2. Basic concepts.** For positive time step  $\Delta t$ , let  $t_k = k\Delta t$ ,  $k = 0, 1, 2, \dots$ . At time  $t_k$ , let particle  $P_i$  of mass  $m_i$  be located at  $\mathbf{x}_{i,k} = (x_{i,k}, y_{i,k}, z_{i,k})$ , have velocity  $\mathbf{v}_{i,k} = (v_{i,k,x}, v_{i,k,y}, v_{i,k,z})$ , and have acceleration  $\mathbf{a}_{i,k} = (a_{i,k,x}, a_{i,k,y}, a_{i,k,z})$ , for  $i = 1, 2, \dots, n$ . Position, velocity, and acceleration are assumed to be related by the fundamental formulas [2]:

$$(2.1) \quad (\mathbf{v}_{i,k+1} + \mathbf{v}_{i,k})/2 = (\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k})/(\Delta t),$$

$$(2.2) \quad \mathbf{a}_{i,k} = (\mathbf{v}_{i,k+1} - \mathbf{v}_{i,k})/(\Delta t).$$

If  $\mathbf{F}_{i,k} = (F_{i,k,x}, F_{i,k,y}, F_{i,k,z})$  is the force acting on  $P_i$  at time  $t_k$ , then force and acceleration are assumed to be related by the discrete dynamical equation

$$(2.3) \quad \mathbf{F}_{i,k} = m_i \mathbf{a}_{i,k}.$$

The work  $W_i$  done by  $\mathbf{F}_{i,k}$  on  $P_i$  from initial time  $t_0$  to terminal time  $t_N$  is defined by

$$(2.4) \quad W_i = \sum_{k=0}^{N-1} [(\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k}) \cdot \mathbf{F}_{i,k}],$$

while the total work  $W$  done on the system from time  $t_0$  to time  $t_N$  is defined by

$$(2.5) \quad W = \sum_{i=1}^n W_i.$$

3. **Conservation of kinetic energy.** From (2.1)–(2.4), it follows that

$$\begin{aligned} W_i &= m_i \sum_{k=0}^{N-1} [(x_{i,k+1} - x_{i,k})a_{i,k,x} + (y_{i,k+1} - y_{i,k})a_{i,k,y} + (z_{i,k+1} - z_{i,k})a_{i,k,z}] \\ &= \frac{1}{2}m_i \sum_{k=0}^{N-1} [(v_{i,k+1,x}^2 - v_{i,k,x}^2) + (v_{i,k+1,y}^2 - v_{i,k,y}^2) + (v_{i,k+1,z}^2 - v_{i,k,z}^2)] \\ &= \frac{1}{2}m_i(v_{i,N,x}^2 + v_{i,N,y}^2 + v_{i,N,z}^2) - \frac{1}{2}m_i(v_{i,0,x}^2 + v_{i,0,y}^2 + v_{i,0,z}^2). \end{aligned}$$

Thus, if the kinetic energy  $K_{i,k}$  of  $P_i$  at  $t_k$  is defined by

$$(3.1) \quad K_{i,k} = \frac{1}{2}m_i(v_{i,k,x}^2 + v_{i,k,y}^2 + v_{i,k,z}^2),$$

then

$$(3.2) \quad W_i = K_{i,N} - K_{i,0}.$$

Finally, if the kinetic energy  $K_k$  of the system at  $t_k$  is defined by

$$(3.3) \quad K_k = \sum_{i=0}^n K_{i,k},$$

then (2.5), (3.2), and (3.3) imply

$$(3.4) \quad W = K_N - K_0,$$

which is called the law of conservation of kinetic energy.

It is interesting to note that (3.4) is valid independently of the specific structure of the forces involved.

4. **The  $n$ -body force law.** In order to simulate Newtonian gravitation and various classical laws of molecular interaction ([1], [5]), we will structure the force between each pair of particles to consist of a component of attraction which behaves like  $p/(r^\alpha)$  and a component of repulsion which behaves like  $q/(r^\beta)$ , where  $p$ ,  $q$ ,  $\alpha$ , and  $\beta$  are nonnegative parameters and  $r$  is the distance between the particles, as follows. Let  $r_{ij,k}$  be the distance between  $P_i$  and  $P_j$  at time  $t_k$ . Then  $F_{i,k}$ , the force exerted on  $P_i$  by  $P_j$ , is defined by

$$(4.1) \quad F_{i,k} = m_i \sum_{j=1; j \neq i}^n \left\{ m_j \left( - \frac{p \sum_{\xi=0}^{\alpha-2} (r_{ij,k}^\xi r_{ij,k+1}^{\alpha-\xi-2})}{r_{ij,k}^{\alpha-1} r_{ij,k+1}^{\alpha-1} (r_{ij,k+1} + r_{ij,k})} + \frac{q \sum_{\xi=0}^{\beta-2} (r_{ij,k}^\xi r_{ij,k+1}^{\beta-\xi-2})}{r_{ij,k}^{\beta-1} r_{ij,k+1}^{\beta-1} (r_{ij,k+1} + r_{ij,k})} \right) (\mathbf{x}_{i,k+1} + \mathbf{x}_{i,k} - \mathbf{x}_{j,k+1} - \mathbf{x}_{j,k}) \right\}.$$

In particular, (4.1) defines discrete Newtonian gravitation when  $p = G, q = 0, \alpha = 2$ , while it defines a force with discrete Lennard-Jones potential when  $\alpha = 7, \beta = 13$ .

**5. Conservation of energy.** Consider now formula (2.5) with force defined by (4.1). In this connection the following lemma will be of value.

**LEMMA.** For  $n \geq 2$ , the following identity is valid:

$$(5.1) \quad \sum_{j=1; j \neq i}^n \sum_{i=1}^n \left[ \frac{m_i m_j \sum_{\xi=0}^{\alpha-2} (r_{ij,k}^\xi r_{ij,k+1}^{\alpha-\xi-2})}{r_{ij,k}^{\alpha-1} r_{ij,k+1}^{\alpha-1} (r_{ij,k+1} + r_{ij,k})} \right. \\ \left. (\mathbf{x}_{i,k+1} + \mathbf{x}_{i,k} - \mathbf{x}_{j,k+1} - \mathbf{x}_{j,k}) \cdot (\mathbf{x}_{i,k+1} - \mathbf{x}_{i,k}) \right] \\ \equiv \sum_{i,j=1; i < j}^n \left\{ m_i m_j \left( \frac{r_{ij,k+1}^{\alpha-1} - r_{ij,k}^{\alpha-1}}{r_{ij,k}^{\alpha-1} r_{ij,k+1}^{\alpha-1}} \right) \right\}.$$

**PROOF.** The proof follows readily by mathematical induction on  $n$ . From (2.5), (4.1), and (5.1), then,

$$W = \sum_{k=0}^{N-1} \sum_{i,j=1; i < j}^n \left\{ m_i m_j \left( -p \frac{r_{ij,k+1}^{\alpha-1} - r_{ij,k}^{\alpha-1}}{r_{ij,k}^{\alpha-1} r_{ij,k+1}^{\alpha-1}} + q \frac{r_{ij,k+1}^{\beta-1} - r_{ij,k}^{\beta-1}}{r_{ij,k}^{\beta-1} r_{ij,k+1}^{\beta-1}} \right) \right\} \\ = \sum_{i,j=1; i < j}^n \left\{ m_i m_j \left[ -p \left( \frac{1}{r_{ij,0}^{\alpha-1}} - \frac{1}{r_{ij,N}^{\alpha-1}} \right) + q \left( \frac{1}{r_{ij,0}^{\beta-1}} - \frac{1}{r_{ij,N}^{\beta-1}} \right) \right] \right\}.$$

Defining the potential energy  $V_{ij,k}$  of the pair  $P_i$  and  $P_j$  at time  $t_k$  by

$$V_{ij,k} = (-p/r_{ij,k}^{\alpha-1} + q/r_{ij,k}^{\beta-1})m_i m_j$$

then yields

$$W = \sum_{i,j=1; i < j}^n V_{ij,0} - \sum_{i,j=1; i < j}^n V_{ij,N}.$$

Defining the potential energy  $V_k$  of the system at  $t_k$  by

$$V_k = \sum_{i,j=1; i < j}^n V_{ij,k}$$

then implies

$$(5.2) \quad W = V_0 - V_N.$$

Finally, elimination of  $W$  between (3.4) and (5.2) yields

$$(5.3) \quad K_N + V_N = K_0 + V_0, \quad N = 0, 1, 2, \dots,$$

which is the classical law of conservation of energy.

**6. Remarks.** Let us note first that the algebraic formulation of this paper

yields other basic classical results. With regard to initial value problems, for example, (2.3) and (4.1) imply

$$(6.1) \quad \sum_{i=1}^n m_i \mathbf{a}_{i,k} = \mathbf{0},$$

so that, from (2.2),

$$(6.2) \quad \sum_{i=1}^n m_i (\mathbf{v}_{i,k+1} - \mathbf{v}_{i,k}) = \mathbf{0}.$$

Summing both sides of (6.2) over  $k$  from 0 to  $s - 1$ , where  $s \geq 1$ , yields

$$(6.3) \quad \sum_{i=1}^n m_i (\mathbf{v}_{i,s} - \mathbf{v}_{i,0}) = \mathbf{0}.$$

Since (6.3) is valid also for  $s = 0$ , then

$$(6.4) \quad \sum_{i=1}^n m_i \mathbf{v}_{i,s} = \mathbf{c}_1, \quad s \geq 0,$$

where  $\mathbf{c}_1$  is a constant vector. Formula (6.4) is, of course, the law of conservation of linear momentum. From (6.4) it then follows that

$$(6.5) \quad \sum_{i=1}^n m_i \left( \frac{\mathbf{v}_{i,s+1} + \mathbf{v}_{i,s}}{2} \right) = \mathbf{c}_1, \quad s \geq 0.$$

Thus, from (2.1),

$$(6.6) \quad \sum_{i=1}^n m_i (\mathbf{x}_{i,s+1} - \mathbf{x}_{i,s}) = (\Delta t) \mathbf{c}_1, \quad s \geq 0.$$

Summing both sides of (6.6) over  $s$  from 0 to  $r - 1$ , for  $r \geq 1$ , implies

$$(6.7) \quad \sum_{i=1}^n m_i (\mathbf{x}_{i,r} - \mathbf{x}_{i,0}) = t_r \mathbf{c}_1.$$

However, (6.7) is valid also for  $r = 0$ , so that

$$(6.8) \quad \sum_{i=1}^n m_i \mathbf{x}_{i,r} = t_r \mathbf{c}_1 + \mathbf{c}_2,$$

where  $\mathbf{c}_2$  is a constant vector. Finally, set  $M = \sum_{i=1}^n m_i$  and let  $\mathbf{X}_r$  be the center of gravity of the system at time  $t_r$ . Then (6.8) implies

$$M \mathbf{X}_r = t_r \mathbf{c}_1 + \mathbf{c}_2,$$

from which it follows that the motion of the centroid is linear.

Finally, note that analogous techniques ([3], [4]) yield the same results of this paper for discrete mechanical systems in which (2.2) is replaced by either

$$(a_{i,k+1} + a_{i,k})/2 = (v_{i,k+1} - v_{i,k})/(\Delta t),$$

or

$$\frac{1}{2}(3a_{i,k} - a_{i,k-1}) = (v_{i,k+1} - v_{i,k})/(\Delta t).$$

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