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ABSTRACT

In previous work, a new numerical method--"discrete mechanics"--was presented which conserved exactly the additive constants of motion. The basic formulae of "discrete mechanics" were originally derived for the case of a separable, radial potential. In the present work, "discrete mechanics" is extended to include nonseparable potentials with separable, radial arguments. Application to the LEPS potential form, common in modeling chemical reactions, is discussed.

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1. Introduction

In the study of a system of particles moving according to the laws of classical mechanics, conservation of energy and angular momentum is of fundamental importance. In previous work [1]-[3], a new numerical method--"discrete mechanics"--was developed which exactly conserved the additive constants of motion. In [1], the basic conservative formulae were obtained for a general separable, radially dependent potential ϕ . In [2], "discrete mechanics" was extended to include anisotropic potentials In [3], the theory was extended to an arbitrary numerical order of approximation.

Although the potentials in fundamental physical interactions are representable by separable, radial forms, certain approximate theories of molecules lead to nonseparable functionalities. A notable example is the London-Eyring-Polanyi-Sato (LEPS) potential form [4], which involves a square-root of a sum of radially dependent functions. This LEPS form is in common use in the study of three-body exchange reactions [5].

In the present work, "discrete mechanics" is extended to the case of a nonseparable potential which has a separable argument. The theory is developed in Section 3, and is applied to the case of the LEPS potential in Section 4.

2. Discrete Mechanics Equations for a Separable Potential

For convenience and completeness, the basic formulae developed in [1], which will be needed below, will now be summarized. For the motion of a system of particles, the "discrete mechanics" formulae of [1] are based upon explicit use of the functionality of the potential ϕ of interaction of a system of particles. Suppose that ϕ is a separable function of the n distances r_i ; i.e., is of the form

$$\phi(r_1,r_2,\ldots,r_n) = \sum_{\ell=0}^{\infty} \phi_1^{(\ell)}(r_1)\phi_2^{(\ell)}(r_2)\ldots\phi_n^{(\ell)}(r_n) \tag{1}$$

Typically r_i is the distance between two particles, although from the theory of [1]-[2] the mathematical form of the succeeding equations below is preserved if r_i is the distance of particle i from the origin, or is equal to the scalar product of two vector distances from the origin. For convenience of notation, assume that r_i denotes the distance of particle i from the origin.

For a given system, let E denote the value of the energy as calculated from the initial conditions and E' the value of the energy calculated from the final conditions at the end of a time step Δt . (In general, primes will denote evaluation at the end of the time step.) For conservation of energy to occur, E and E' must have the same value, or

$$\Delta E = E' - E \tag{2a}$$

$$= 0 \tag{2b}$$

From equation (5.50) of [1], ΔE can be written

$$\Delta E = \Delta T_1 + \Delta T_2 + \ldots + \Delta T_n + \Delta\phi \tag{3}$$

where

$$\Delta\phi = \phi(r_1', r_2', \ldots, r_n') - \phi(r_1, r_2, \ldots, r_n) \tag{4}$$

is the change of potential over the time step, and ΔT_i is the i-th component of the change in the total kinetic energy T over the time step. The explicit forms of the ΔT_i in terms of the numerical solution will vary with the order of approximation and the identification of the r_i. For example, for the low-order discrete mechanics of [1], and r_i the distance of particle i from the origin (equation (5.24) of [1]),

$$\Delta T_i = \vec{F}_i^{*} \cdot \Delta\vec{r}_i \tag{5}$$

where $\vec{F}_i^{*}$ is the discrete mechanics' "force", and

$$\Delta\vec{r}_i = \vec{r}_i' - \vec{r}_i \tag{6}$$

Here $\vec{r}_i$ denotes the vector radius of particle i from the origin.

Whatever the explicit form of ΔT_i in terms of the numerical method, from equation (5.62) of [1], if ϕ is given by equation (1) above, then

$$\Delta T_i = -\sum_{\ell=0}^{\infty} \Delta\tilde{\phi}_i^{(\ell)} \qquad (i=1,2,\ldots,n) \tag{7}$$

where $\Delta\tilde{\phi}_i^{(\ell)}$ is given by the symmetrized product

$$\Delta\tilde{\phi}_i^{(\ell)} = \frac{\phi_i^{(\ell)\prime} - \phi_i^{(\ell)}}{n} \sum_{k=0}^{n-1} \frac{1}{\binom{n-1}{k}} \sum_{1}^{\binom{n-1}{k}} \left(\prod_{s=1}^{k} \phi_{i_s}^{(\ell)\prime}\right)\left(\prod_{s=k+1}^{n-1} \phi_{i_s}^{(\ell)}\right) \tag{8}$$

$$(i=1,2,\ldots,n;\ i_s \neq i)$$

In equation (8),

$$\phi_m^{(\ell)\prime} = \phi_m^{(\ell)}(r_m')$$

$$\phi_m^{(\ell)} = \phi_m^{(\ell)}(r_m)$$

and the second sum is over all possible combinations of products of the n-1 functions $\phi_{i_s}^{(\ell)}$, for which $i_s \neq i$, and of which k are evaluated at the new arguments r_{i_s}' and n-1-k at the old arguments r_{i_s}.

Examples of equation (8) are as follows: For n=1,

$$\Delta\tilde{\phi}_1^{(\ell)} = \phi_1^{(\ell)\prime} - \phi_1^{(\ell)} ; \tag{9}$$

for n=2,

$$\Delta\tilde{\phi}_1^{(\ell)} = \frac{\phi_1^{(\ell)\prime} - \phi_1^{(\ell)}}{2}(\phi_2^{(\ell)\prime} + \phi_2^{(\ell)}) \tag{10a}$$

$$\Delta\tilde{\phi}_2^{(\ell)} = \frac{\phi_2^{(\ell)\prime} - \phi_2^{(\ell)}}{2}(\phi_1^{(\ell)\prime} + \phi_1^{(\ell)}) ; \tag{10b}$$

and, for n=3,

$$\Delta\tilde{\phi}_1^{(\ell)} = \frac{\phi_2^{(\ell)\prime} - \phi_2^{(\ell)}}{3}\left[\phi_2^{(\ell)\prime}\phi_3^{(\ell)\prime} + \frac{1}{2}(\phi_2^{(\ell)\prime}\phi_3^{(\ell)} + \phi_2^{(\ell)}\phi_3^{(\ell)\prime}) + \phi_2^{(\ell)}\phi_3^{(\ell)}\right] \tag{11}$$

The formulae for $\Delta\tilde{\phi}_2^{(\ell)}$ and $\Delta\tilde{\phi}_3^{(\ell)}$ are obtained from equation (11) via cyclic permutation of the indices 1, 2, 3.

As an illustration, the use of the above formulae for ΔT_i and $\Delta\tilde{\phi}_i^{(\ell)}$ will be shown for the low-order discrete mechanics of [1]. For this case equation (5) holds. In [1] it was found that the

"force" $\vec{F}_i^*$ must lie along $\vec{r}_i' + \vec{r}_i$ for conservation of angular momentum to occur. This condition, along with equation (5), leads to

$$\vec{F}_i^* = \frac{\Delta T_i}{\Delta r_i} \frac{\vec{r}_i' + \vec{r}_i}{r_i' + r_i} \tag{12}$$

where

$$\Delta r_i = r_i' - r_i \tag{13}$$

Substitution for ΔT_i via equation (7) now gives

$$\vec{F}_i^* = \sum_{\ell=0}^{\infty} \frac{\Delta \tilde{\phi}_i^{(\ell)}}{\Delta r_i} \frac{\vec{r}_i' + \vec{r}_i}{r_i' + r_i} \tag{14}$$

Equation (14) for $\vec{F}_i^*$, coupled with equations (5.3) of [1], are all that is needed to numerically calculate the trajectory of motion.

For example, if $\vec{r}_i$ is the vector distance of particle i of mass m_i from the origin, and $\vec{v}_i$ is the velocity of the particle, i.e.,

$$\vec{v}_i = \frac{d\vec{r}_i}{dt} \tag{15}$$

then the new position and velocities are determined via the equations

$$\vec{r}_i' = \vec{r}_i + \vec{v}_i \, \Delta t + \frac{\vec{F}_i^*}{m_i} \frac{(\Delta t)^2}{2} \tag{16a}$$

$$\vec{v}_i' = \vec{v}_i + \frac{\vec{F}_i^*}{m_i} \Delta t \tag{16b}$$

where Δt is the time step and F_i^* is given by equation (14).

3. Discrete Mechanics Equations for Nonseparable Potentials

In what follows, the discrete mechanics equations will be developed for the case of a nonseparable potential function $\phi(u)$, where u is a separable argument. For heuristic reasons, u will be limited to the cases $u = r_1 r_2$ and $u = r_1 + r_2$ in Sections 3.A and 3.B, respectively. The results are then generalized in Section 3.C.

In each of the subsections below, $\phi(u)$ is assumed to be a general function of u, and is not required to be separable. For example,

$$\phi(u) = e^u$$

or

$$\phi(u) = u^{1/2}$$

are possible choices.

A. Product of Radii Argument

Suppose that $\phi(u)$ is a given, nonseparable function, $n=2$, and

$$u = r_1 r_2 \tag{17}$$

The problem is to find the forms of ΔT_1 and ΔT_2 so that equation (2b) is satisfied. While it is entirely possible to derive the results below via the rigorous approach of the method of undetermined coefficients used in [1], a heuristic argument which is easier to follow will be presented here. The solution, of course, is easily verified to be rigorous.

Since $\vec{F}_1^*$ and $\vec{F}_2^*$ are related to ΔT_1 and ΔT_2 via equation (12), discovery of their forms will lead to those for the ΔT_i. Now the $\vec{F}_i^*$ must reduce to the exact forces $\vec{F}_i$ as $\Delta t \to 0$.

Therefore the form of the exact forces will give an indication of the form of the $\vec{F}_i^*$. From the laws of mechanics, $\vec{F}_i$ is given by the $\vec{r}_i$ gradient of the potential:

$$\vec{F}_i = - \frac{\partial \phi}{\partial \vec{r}_i} \tag{18}$$

Assuming that $\phi = \phi(u)$, with u given by equation (17), then, by the chain-rule,

$$\vec{F}_i = - \frac{d\phi}{du} \frac{\partial u}{\partial \vec{r}_i} \tag{19a}$$

$$= - \frac{d\phi}{du} \frac{du}{dr_i} \frac{\vec{r}_i}{r_i} \tag{19b}$$

Using equation (17),

$$\vec{F}_i = - \frac{d\phi}{du} r_2 \frac{\vec{r}_1}{r_1} \tag{20a}$$

$$\vec{F}_2 = - \frac{d\phi}{du} r_1 \frac{\vec{r}_2}{r_2} \tag{20b}$$

Both $\vec{F}_1^*$ and $\vec{F}_2^*$ as given by equation (12) must reduce to equations (20) as $\Delta t \to 0$. This leads (via equations (12) and (20)) to the qualitative statements that

$$\Delta T_1 = - \frac{d\phi}{du} r_2 \Delta r_1 + O[(\Delta t)^2] \tag{21a}$$

$$\Delta T_2 = - \frac{d\phi}{du} r_1 \Delta r_2 + O[(\Delta t)^2] \tag{21b}$$

Replacing the derivative with a difference quotient and symmetrizing, reasonable forms for the ΔT_i are given by

$$\Delta T_1 = - \left(\frac{r_2' + r_2}{2}\right) \frac{\Delta\phi}{\Delta u} \Delta r_1 \tag{22a}$$

$$\Delta T_2 = - \left(\frac{r_1' + r_1}{2}\right) \frac{\Delta\phi}{\Delta u} \Delta r_2 \tag{22b}$$

It is easy to verify that equations (22) for the ΔT_i lead to conservation of energy via equations (2):

$$\Delta T_1 + \Delta T_2 = - \frac{\Delta\phi}{\Delta u} \left(\frac{r_2' + r_2}{2}\right) (r_1' - r_1) - \frac{\Delta\phi}{\Delta u} \left(\frac{r_1' + r_1}{2}\right) (r_2' - r_2) \tag{23a}$$

$$= - \frac{1}{2} \frac{\Delta\phi}{\Delta u} (r_2' r_1' + r_2 r_1' - r_2' r_1 - r_2 r_1 + r_1' r_2' + r_1 r_2' - r_1' r_2 - r_1 r_2) \tag{23b}$$

$$= - \frac{\Delta\phi}{\Delta u} (r_1' r_2' - r_1 r_2) \tag{23c}$$

Since u is given by equation (17),

$$\Delta u = u' - u \tag{24a}$$

$$= r_1' r_2' - r_1 r_2 \tag{24b}$$

and equation (23c) becomes

$$\Delta T_1 + \Delta T_2 = - \Delta\phi \tag{25}$$

Equation (25) implies $\Delta E = 0$ in equation (2b) and energy is conserved.

As mentioned above, a more rigorous derivation of the ΔT_i also leads to equations (22), so that these formulae are not limited to the low-order case. Conservation of angular momentum occurs, however, due to the explicit direction of the forces $\vec{F}_i^*$, which varies with the order of approximation [3]. Luckily conservation of angular momentum as given previously ([1], [3]) is free from explicit dependence on the form of ϕ.

B. Sum of Radii Argument

In Section 3.A above, the product form for u was discussed. Suppose now that the argument u of ϕ is given by

$$u = r_1 + r_2 \tag{26}$$

Following the approach of Section 3.A, the exact forces $\vec{F}_i$ are given by

$$F_i = - \frac{d\phi}{du} \frac{du}{dr_i} \frac{\vec{r}_i}{r_i} \tag{27a}$$

$$= - \frac{d\phi}{du} \frac{\vec{r}_i}{r_i} \qquad (i=1,2) \tag{27b}$$

Comparison of equations (12) and (27) yields

$$\Delta T_i = - \frac{d\phi}{du} \Delta r_i + O[(\Delta t)^2] \qquad (i=1,2) \tag{28}$$

leading to the guesses

$$\Delta T_i = - \frac{\Delta\phi}{\Delta u} \Delta r_i \tag{29}$$

As in Section 3.A above, it is easy to verify equations (29) for the ΔT_i lead to conservation of energy:

$$\Delta T_1 + \Delta T_2 = - \frac{\Delta\phi}{\Delta u} \Delta r_1 - \frac{\Delta\phi}{\Delta u} \Delta r_2 \tag{30a}$$

$$= - \frac{\Delta\phi}{\Delta u} (r_1'-r_1+r_2'-r_2) \tag{30b}$$

$$= - \frac{\Delta\phi}{\Delta u} (r_1'+r_2'-r_1-r_2) \tag{30c}$$

$$= - \frac{\Delta\phi}{\Delta u} (u'-u) \tag{30d}$$

$$= - \frac{\Delta\phi}{\Delta u} \Delta u \tag{30e}$$

$$= - \Delta\phi \tag{30f}$$

giving $\Delta E = 0$ in equation (2b).

With the ΔT_i given by equation (29), the discrete mechanics forces $\vec{F}_i^*$ from equation (12) become

$$\vec{F}_i^* = - \frac{\Delta\phi}{\Delta u} \frac{\vec{r}_i' + \vec{r}_i}{r_i' + r_i} \quad (i=1,2) \tag{31}$$

As in Section 3.A, equations (29), could be derived rigorously, and are valid for all orders of approximations; conversely, equations (31) are valid only for discrete mechanics of [1].

C. General Separable Argument

Except for the factor $\Delta\phi/\Delta u$, equation (29) for the ΔT_i resembles equation (9), and equations (22) resemble equations (10), if the radii r_1 and r_2 are treated similar to the ϕ_i of Section 2. This suggests, via equation (8), a general form for ΔT_i .

Suppose

$$\phi(r_1, r_2, \ldots, r_n) = \phi(u) \tag{32}$$

and the argument u is given by the separable form

$$u = \sum_{\ell=0}^{\infty} u_1^{(\ell)}(r_1) u_2^{(\ell)}(r_2) \ldots u_n^{(\ell)}(r_n) \tag{33}$$

where the $u_i^{(\ell)}$ are arbitrary functions. Then ΔT_i is given by

$$\Delta T_i = - \frac{\Delta\phi}{\Delta u} \sum_{\ell=0}^{\infty} \Delta\tilde{u}_i \quad (i=1,2,\ldots,n) \tag{34}$$

where

$$\Delta\tilde{u}_i = \frac{u_i^{(\ell)\prime} - u_i^{(\ell)}}{n} \sum_{k=0}^{n-1} \frac{1}{\binom{n-1}{k}} \sum_{\binom{n-1}{k}} \left(\prod_{s=1}^{k} u_{i_s}^{(\ell)\prime} \right)$$

$$\times \left(\prod_{s=k+1}^{n-1} u_{i_s}^{(\ell)} \right) \qquad (35)$$

$$(i=1,2,\ldots,n;\ i_s \neq i)$$

similar to equation (8) with $u_m^{(\ell)}$ substituted for $\phi_m^{(\ell)}$.

Since $\Delta\phi/\Delta u$ in equation (34) is a constant factor of each ΔT_i, conservation of energy is easily shown. Conservation in Section 2 gives, by substitution of the separable form of u for ϕ,

$$\Delta u = \sum_{i=1}^{n} \sum_{\ell=0}^{\infty} \Delta\tilde{u}_i^{(\ell)} \qquad (36)$$

Thus, using equations (34) and (36)

$$\Delta T_1 + \Delta T_2 + \ldots + \Delta T_n = -\frac{\Delta\phi}{\Delta u} \sum_{i=1}^{n} \sum_{\ell=0}^{\infty} \Delta\tilde{u}_i \qquad (37a)$$

$$= -\frac{\Delta\phi}{\Delta u} (\Delta u) \qquad (37b)$$

$$= -\Delta\phi \qquad (37c)$$

so that $\Delta E = 0$ in equation (2b).

For $n=2$, equations (22) result when

$$u = u_1^{(0)}(r_1) u_2^{(0)}(r_2) \qquad (38)$$

and

$$u_1^{(0)}(r_1) = r_1 \tag{39a}$$

$$u_2^{(0)}(r_2) = r_2 \tag{39b}$$

Similarly, equation (29) is obtained from equations (34) and (35) for the case

$$u = u_1^{(0)}(r_1)u_2^{(0)}(r_2) + u_1^{(1)}(r_1)u_2^{(1)}(r_2) \tag{40}$$

where

$$u_1^{(0)}(r_1) = r_1 \tag{41a}$$

$$u_2^{(0)}(r_2) = 1 \tag{41b}$$

and

$$u_1^{(1)}(r_1) = 1 \tag{42a}$$

$$u_2^{(1)}(r_2) = r_2 \tag{42b}$$

4. Application to the LEPS Potential

The London-Eyring-Polanyi-Sato (LEPS) potential form [4] for the interaction of three particles is frequently used in the qualitative theoretical study of chemical reactions [5]. For this potential $\phi(r_1,r_2,r_3)$, the r_i are the distances between the three particles

$$r_1 = \rho_{12} \tag{43a}$$

$$r_2 = \rho_{23} \tag{43b}$$

$$r_3 = \rho_{13} \tag{43c}$$

and has the form

$$\phi(r_1,r_2,r_3) = Q_1 + Q_2 + Q_3$$

$$- [J_1^2+J_2^2+J_3^2-J_1J_2-J_1J_3-J_2J_3]^{1/2} \tag{44}$$

In equation (44),

$$Q_i = Q_i(r_i) \qquad (i=1,2,3) \tag{45a}$$

$$J_i = J_i(r_i) \tag{45b}$$

are two-body potentials, which may be described by standard forms.

The part of ϕ represented by the Q_i is handled easily by the formulae of Section 2; the last term involving the square-root is, however, nonseparable and requires the use of equations (34) and (35). Concentrating attention on the square-root term, let

$$\phi = [J_1^2+J_2^2+J_3^2-J_1J_2-J_1J_3-J_2J_3]^{1/2} \tag{46}$$

and

$$u = J_1^2 + J_2^2 + J_3^2 - J_1J_2 - J_1J_3 - J_2J_3 \tag{47}$$

For the first three terms in u, $n=1$ but the subscript on the r varies. For the last three terms, $n=2$ since two radial dependences are involved. Thus, via equation (35),

$$\Delta\tilde{u}_1 = (J_1')^2 - J_1^2 - \frac{J_1'-J_1}{2}(J_2'+J_2) - \frac{J_1'-J_1}{2}(J_3'+J_3) \tag{48a}$$

$$= (J_1'-J_1)(J_1'+J_1 - \frac{J_2'+J_2}{2} - \frac{J_3'+J_3}{2}) \tag{48b}$$

where

$$J_i' = J_i(r_i') \tag{49}$$

with r_i' being the value of r_i at the end of the time step. Similarly,

$$\Delta\tilde{u}_2 = (J_2'-J_2)(J_2'+J_2 - \frac{J_1'+J_1}{2} - \frac{J_3'+J_3}{2}) \tag{50a}$$

$$\Delta\tilde{u}_3 = (J_3'-J_3)(J_3'+J_3 - \frac{J_1'+J_1}{2} - \frac{J_2'+J_2}{2}) \tag{50b}$$

Finally, using equation (9) for the Q_i terms in equation (44), and via equation (34) for the contribution from ϕ,

$$\Delta T_1 = -(Q_1'-Q_1) - \frac{\phi'-\phi}{u'-u}\Delta\tilde{u}_1 \tag{51a}$$

$$= -(Q_1'-Q_1) - \frac{\phi'-\phi}{u'-u}(J_1'-J_1) \times (J_1'+J_1 - \frac{J_2'+J_2}{2} - \frac{J_3'+J_3}{2}) \tag{51b}$$

where

$$\phi' = \phi(u') \tag{52a}$$

$$u' = u(J_1', J_2', J_3') \tag{52b}$$

and

$$Q_i' = Q_i(r_i') \tag{53}$$

Similar results for ΔT_2 and ΔT_3 are obtained from equations (51) via cyclic permutation of the indices 1, 2, 3.

When applied to the low-order discrete mechanics of [1], equations (51) lead, via equation (12), to the discrete mechanics "forces"

$$\vec{F}_1^* = -\left[\frac{Q_1'-Q_1}{r_1'-r_1} + \frac{\phi'-\phi}{u'-u}\,\frac{J_1'-J_1}{r_1'-r_1} \times \left(J_1'+J_1 - \frac{J_2'+J_2}{2} - \frac{J_3'+J_3}{2}\right)\right] \frac{\vec{r}_1'+\vec{r}_1}{r_1'+r_1} \tag{54a}$$

$$\vec{F}_2^* = -\left[\frac{Q_2'-Q_2}{r_2'-r_2} + \frac{\phi'-\phi}{u'-u}\,\frac{J_2'-J_2}{r_2'-r_2} \times \left(J_2'+J_2 - \frac{J_1'+J_1}{2} - \frac{J_3'+J_3}{2}\right)\right] \frac{\vec{r}_2'+\vec{r}_2}{r_2'+r_2} \tag{54b}$$

$$\vec{F}_3^* = -\left[\frac{Q_3'-Q_3}{r_3'-r_3} + \frac{\phi'-\phi}{u'-u}\,\frac{J_3'-J_3}{r_3'-r_3} \times \left(J_3'+J_3 - \frac{J_1'+J_1}{2} - \frac{J_2'+J_2}{2}\right)\right] \frac{\vec{r}_3'+\vec{r}_3}{r_3'+r_3} \tag{54c}$$

As a comparison, the exact forces required by conventional numerical methods may be obtained by differentiation of equation (44):

$$\vec{F}_i = -\frac{\partial \phi}{\partial \vec{r}_i} \tag{55a}$$

$$= -\frac{\partial Q_i}{\partial \vec{r}_i} - \frac{\partial \phi}{\partial \vec{r}_i} \tag{55b}$$

$$= -\left[\frac{dQ_i}{dr_i} + \frac{d\phi}{du}\frac{du}{dr_i}\right]\frac{\vec{r}_i}{r_i} \tag{55c}$$

Since u is given by equation (47), then, e.g.,

$$\frac{du}{dr_1} = 2J_1\frac{dJ_1}{dr_1} - J_2\frac{dJ_1}{dr_1} - J_3\frac{dJ_1}{dr_1} \tag{56a}$$

$$= [2J_1 - J_2 - J_3]\frac{dJ_1}{dr_1} \tag{56b}$$

Since $\phi = u^{1/2}$,

$$\frac{d\phi}{du} = \frac{1}{2}\frac{1}{\phi} \tag{57}$$

Combining equations (55c), (56) and (57), the formula for, e.g., $\vec{F}_1$ is given by

$$\vec{F}_1 = -\left[\frac{dQ_1}{dr_1} + \frac{1}{2\phi}(2J_1 - J_2 - J_3)\frac{dJ_1}{dr_1}\right]\frac{\vec{r}_1}{r_1} \tag{58}$$

Several comments can be made concerning a comparison of equations (54a) and (58). Firstly, it is clear $\vec{F}_1^* \to \vec{F}_1$ as $\Delta t \to 0$. Secondly, the amount of new information per step that is required to evaluate $\vec{F}_1^*$ is: Q_1' , J_1' , J_2' , J_3' , and the derived quantities u' and ϕ' . For $\vec{F}_1$, the corresponding information is dQ_1/dr_1,, J_1 , J_2 , J_3 , dJ_1/dr_1 , and the derived quantities u and ϕ . Therefore, since the dominant factor in computing time is usually the evaluation of the complicated functions and derivatives of Q_i and J_i , the discrete mechanics "forces" $\vec{F}_i^*$ require slightly less computational effort to find than the exact forces $\vec{F}_i$.

5. Conclusion

The energy and angular momentum conserving formulae of [1]-[3] have been extended to include the class of nonseparable potentials with separable arguments. Application was made to the case of the LEPS potential commonly used in studies of exchange reactions. By recursive use of the formulae of Section 3, almost any potential can be handled which is at the lowest level separable. The formulae of this work, coupled with those of Section 2, cover all known forms of model potentials in use in physics at the present time. Although formulae for certain functionalities, such as $\phi(r_1,r_2) = r_1^{r_2}$ have not yet been developed, such functionalities fortunately do not occur in the treatment of physical problems.

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15. Supplementary Notes

16. Abstracts

In previous work, a new numerical method--"discrete mechanics"--was presented which conserved exactly the additive constants of motion. The basic formulae of "discrete mechanics" were originally derived for the case of a separable, radial potential. In the present work, "discrete mechanics" is extended to include nonseparable potentials with separable, radial arguments. Application to the LEPS potential form, common in modeling chemical reactions, is discussed.

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