Discrete dynamics versus analytic dynamics

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For discrete classical Molecular dynamics obtained by the "Verlet" algorithm (VA) with the time increment h there exists a shadow Hamiltonian $\tilde{H}$ with energy $\tilde{E}(h)$, for which the discrete particle positions lie on the analytic trajectories for $\tilde{H}$. Here, we proof that there, independent of such an analytic analogy, exists an exact hidden energy invariance E^* for VA dynamics. The fact that the discrete VA dynamics has the same invariances as Newtonian dynamics raises the question, which of the formulations that are correct, or alternatively, the most appropriate formulation of classical dynamics. In this context the relation between the discrete VA dynamics and the (general) discrete dynamics investigated by Lee [Phys. Lett. B **122**, 217 (1983)] is presented and discussed.
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I. INTRODUCTION

Molecular Dynamics (MD) generates the time evolution of N classical mechanical particles by discrete time propagation. Almost all the MD are obtained by the "Verlet" algorithm (VA)[1] where a new position $\mathbf{r}_i(t+\delta t)$ of the ith particle with mass m_i at time $t+\delta t$ is obtained from the force $\mathbf{f}_i(t)$ and the two last discrete positions

$$\mathbf{r}_i(t+\delta t) = 2\mathbf{r}_i(t) - \mathbf{r}_i(t-\delta t) + \frac{\delta t^2}{m_i}\mathbf{f}_i(t). \qquad (1)$$

The algorithm is the central-difference expression for the mass times the acceleration of the particle which equals the force $\mathbf{f}_i$, and it appears in the literature with different names (Verlet, leap-frog, velocity Verlet, etc.).[2] The algorithm is time reversible and symplectic, and the different reformulations of the algorithm do not change the discrete time evolution and the physics obtained by the VA dynamics.

Mathematical investigations[3–5] have proved the existence of a shadow Hamiltonian $\tilde{H}$[6] for symplectic algorithms. The proof is obtained by an asymptotic expansion, but the series for the shadow Hamiltonian does not converge in the general case. For a review of the asymptotic expansion, its convergence, and optimal truncation, see Ref. 7. Only the harmonic approximation, $E(1)$ of the first term in this expansion is known explicitly.[2,6] But inclusion of $E(1)$ in the traditional obtained zero order energy for MD systems with Lennard-Jones (LJ) particles reduces the fluctuation in the energy by a factor of hundred for traditional values of δt^2 and makes it possible to obtain the shadow energy, $\tilde{E}$ of the analytic dynamics with high precision.

The VA algorithm deviates, however, from all other algorithms for classical dynamics by that *momenta are not dynamical variables*. Furthermore, the discrete VA dynamics for a harmonic oscillator (DDHO), which can be solved exactly, reveals that the DDHO not only has an asymptotic expansion with an underlying analytic shadow Hamiltonian. But the DDHO dynamics also has a *(hidden) energy invariance*, E^* which, independent of an existence of an analytic shadow Hamiltonian, is conserved step by step during the discrete time evolution. Below we show that this hidden invariance is a general quality of the discrete VA dynamics, independent of the existence of a shadow Hamiltonian, and that the discrete VA dynamics has the same qualities and conserved invariances as analytic Newtonian dynamics. In order to prove the existence of a hidden energy invariance we must not make use of any analytic tools. This might seem to be a hopeless agenda, but on the other hand the exact solution for a discrete harmonic oscillator[6] makes no use of analyticity and the exact solution has an energy invariance E^* which in the analytic limit is equal to the energy of analytic Newtonian dynamics.

II. THE HIDDEN ENERGY INVARIANCE

The kinetic energy in analytic dynamics is obtained from the momenta. The positions in Eq. (1) are the only dynamic variables in the discrete VA dynamics, i.e., the momenta, $\mathbf{p}_i$, are not. Consequently, an expression for the total momentum of the system requires a choice of an expression for the momentum $\mathbf{p}_i$ of the ith particle in terms of its positions. The sentences "momenta," "energy," "potential energy," "kinetic energy," and "work" should be given by quotations in discrete VA dynamics to underline the fact that the N objects in the discrete dynamics only exercise mutual "irritations" or forces $\mathbf{f}_i(t_n)$ at their positions at the discrete time $t_n = n\delta t$. With the definition of the momenta

$$\mathbf{p}_i(t_{n-1}, t_n) \equiv m_i \frac{\mathbf{r}_i(t_n) - \mathbf{r}_i(t_{n-1})}{\delta t} \qquad (2)$$

it follows immediately from the algorithm that the total momentum and angular momentum are conserved for conservative systems with $\sum_i^N \mathbf{f}_i(t) = 0$[8]. But the momenta and thereby the "kinetic energies" appear *asynchronous* with the discrete positions and they are not a function of a single set of the discrete positions.

The proof of an invariance, equivalent to the conserved energy in the analytic dynamics is more difficult, but it can be obtained by proving that there exists a hidden "energy"

invariance, E^*, of the N objects' dynamics with the change $\delta E_n^* = 0$ by the discrete step which brings the N positions $\mathbf{R}_n$ with the forces $\mathbf{F}_n$ at time t_n to $\mathbf{R}_{n+1}$ at t_{n+1}.

For simplicity consider N particles with equal masses $m_i = m$, and with the mass included in the discrete time increment, i.e., with $h \equiv \frac{\delta t}{\sqrt{m}}$. A step with discrete dynamics changes the "kinetic energy" of the system by δK^* and its ability, δU^*, to perform a "work," $\delta U^* = -W^*$. Since the momenta and thereby the kinetic energy is given by two sets of positions, a change in kinetic energy is given by three consecutive sets of positions. The proof is obtained by considering two consecutive time steps. A new set of positions, $\mathbf{R}_{n+1}$ is obtained at the nth time step from the two previous sets, $\mathbf{R}_{n-1}$, $\mathbf{R}_n$ and the forces $\mathbf{F}_n$, by which the change in the "kinetic energy" can be defined as

$$\delta K_n^* \equiv \frac{1}{2}\left(\frac{\mathbf{R}_{n+1} - \mathbf{R}_n}{h}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{R}_n - \mathbf{R}_{n-1}}{h}\right)^2. \tag{3}$$

The definition of the change in the kinetic energy for discrete VA dynamics is consistent with the definition of the momenta, Eq. (2).

The forces $\mathbf{F}_n$ bring the N particles to the positions $\mathbf{R}_{n+1}$ and with a change in the ability, δU_n^*, to perform a "work," $\delta U_n^* = -W_n^*$. For the two steps we define the total change

$$2\delta U_n^* = -2W_n^* \equiv -\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_{n-1}) \tag{4}$$

and the discrete dynamics obeys the relation

$$\delta U_n^* + \delta K_n^* = 0. \tag{5}$$

The proof starts by noticing that if one instead of the (NVE) dynamics, obtained by Eq. (1) with a constant time increment h, adjust the $(n+1)$th time increment h_n so $W = 0$, one obtains a geodesic step (NVU)[9] to the positions $\mathbf{R}_{n+1}(\mathrm{U})$ which differs from $\mathbf{R}_{n+1}$. If

$$-2W(\mathrm{U})_n = -\mathbf{F}_n \cdot (\mathbf{R}_{n+1}(\mathrm{U}) - \mathbf{R}_{n-1}) = 0 \tag{6}$$

is inserted in the Verlet algorithm; Eq. (1)

$$\mathbf{R}_{n+1}(\mathrm{U}) = 2\mathbf{R}_n - \mathbf{R}_{n-1} + h_n^2 \mathbf{F}_n, \tag{7}$$

one obtains an expression for h_n^2 at the NVU step at time t_n[9]

$$h_n^2 = -2\frac{\mathbf{F}_n \cdot (\mathbf{R}_n - \mathbf{R}_{n-1})}{\mathbf{F}_n^2}. \tag{8}$$

That is, instead of propagating the system the nth step with the constant time increment h, the increment h_n is adjusted to ensure that the system ability to perform a work is unchanged.

The NVU step at time t_n updates the position to $\mathbf{R}_{n+1}(\mathrm{U})$ and with the geodesic invariance: the constant length of the steps[9]

$$(\mathbf{R}_{n+1}(\mathrm{U}) - \mathbf{R}_n)^2 = (\mathbf{R}_n - \mathbf{R}_{n-1})^2, \tag{9}$$

which is obtained by rearranging and squaring Eq. (7)

$$(\mathbf{R}_{n+1}(\mathrm{U}) - \mathbf{R}_n)^2 = \left(\mathbf{R}_n - \mathbf{R}_{n-1} - 2\frac{\mathbf{F}_n \cdot (\mathbf{R}_n - \mathbf{R}_{n-1})}{\mathbf{F}_n^2}\mathbf{F}_n\right)^2 \tag{10}$$

$$= (\mathbf{R}_n - \mathbf{R}_{n-1})^2, \tag{11}$$

i.e., with the change in "kinetic energy"

$$\delta K(\mathrm{U})_n = \frac{1}{2}\left(\frac{\mathbf{R}_{n+1}(\mathrm{U}) - \mathbf{R}_n}{h}\right)^2 - \frac{1}{2}\left(\frac{\mathbf{R}_n - \mathbf{R}_{n-1}}{h}\right)^2 = 0. \tag{12}$$

So the NVU step to $\mathbf{R}_{n+1}(\mathrm{U})$ obeys

$$\delta U(\mathrm{U})_n = \delta K(\mathrm{U})_n = 0. \tag{13}$$

We are now able to proof the existence of an "energy" invariance (Eq. (5)) by the VA dynamics, Eq. (1). The proof can, e.g., be obtained by deriving the difference between the NVU and the NVE step at t_n. The new positions $\mathbf{R}_{n+1}$ and $\mathbf{R}_{n+1}(\mathrm{U})$ are both obtained from $\mathbf{R}_{n-1}$, $\mathbf{R}_n$, and $\mathbf{F}_n$, but with different time increments. With NVE

$$\begin{aligned} 2\delta U_n^* = -2W_n^* &= -\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_{n-1}) \\ &= -\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_{n+1}(\mathrm{U}) \\ &\quad + \mathbf{R}_{n+1}(\mathrm{U}) - \mathbf{R}_{n-1}) \\ &= -\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_{n+1}(\mathrm{U})). \end{aligned} \tag{14}$$

The difference $\mathbf{R}_{n+1} - \mathbf{R}_{n+1}(\mathrm{U})$ can be obtained from the Verlet algorithm, Eq. (1), and the NVU algorithm, Eqs. (7) and (8), and gives

$$2\delta U_n^* = -2W_n^* = -\big(h^2\mathbf{F}_n^2 + 2\mathbf{F}_n \cdot (\mathbf{R}_n - \mathbf{R}_{n-1})\big). \tag{15}$$

The change in the "kinetic energy" is obtained from the NVE algorithm Eq. (1)

$$\begin{aligned} 2\delta K_n^* &= \left(\frac{\mathbf{R}_{n+1} - \mathbf{R}_n}{h}\right)^2 - \left(\frac{\mathbf{R}_n - \mathbf{R}_{n-1}}{h}\right)^2 \\ &= \frac{(\mathbf{R}_n - \mathbf{R}_{n-1})^2 + h^4\mathbf{F}_n^2 + 2h^2\mathbf{F}_n \cdot (\mathbf{R}_n - \mathbf{R}_{n-1})}{h^2} \\ &\quad - \left(\frac{\mathbf{R}_n - \mathbf{R}_{n-1}}{h}\right)^2 \\ &= h^2\mathbf{F}_n^2 + 2\mathbf{F}_n \cdot (\mathbf{R}_n - \mathbf{R}_{n-1}) \end{aligned} \tag{16}$$

and Eq. (5) for the discrete dynamics is obtained from Eqs. (15) and (16).

The change in kinetic energy in discrete dynamics must necessarily be obtained from two consecutive steps and the change in the systems ability to perform a work is consistently obtained from the same sets of positions. But, by eliminating $\mathbf{R}_{n-1}$ in Eq. (4), one obtains an expression for the change in the ability per time step, δU_n^*

$$\begin{aligned} \delta U_n^* &= -\frac{1}{2}\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_{n-1}) \\ &= -\mathbf{F}_n \cdot (\mathbf{R}_{n+1} - \mathbf{R}_n) + \frac{h^2}{2}\mathbf{F}_n^2. \end{aligned} \tag{17}$$

In the Newtonian dynamics the existence of a potential energy state function, $U(\mathbf{R})$, is ensured by that the total work done around any closed circuit from $\mathbf{R}$ is zero.[10] The VA dynamics is started from two sets of positions $\mathbf{R}_0$ and $\mathbf{R}_1$, and the time increment h. The ability to perform a discrete work $U^*(\mathbf{R})$ is also a state function and it plays the same role as the

potential energy $U(\mathbf{R})$ for analytic Newtonian dynamics. Consider any discrete closed sequence of positions generated with VA dynamics with the time increment h and which starts and ends with the same two configuration $\mathbf{R}_0$ and $\mathbf{R}_1$. The total change in the kinetic energy is

$$\sum_{i=1}^{i=n} \delta K_i^* = \frac{(\mathbf{R}_2-\mathbf{R}_1)^2}{h} - \frac{(\mathbf{R}_1-\mathbf{R}_0)^2}{h} + \frac{(\mathbf{R}_3-\mathbf{R}_2)^2}{h} - \frac{(\mathbf{R}_2-\mathbf{R}_1)^2}{h} + \ldots + \frac{(\mathbf{R}_1-\mathbf{R}_0)^2}{h} = 0. \quad (18)$$

The start ability is $U^*(\mathbf{R}_1)$, and since all the terms in $\sum_{i=1}^{i=n}(\delta U_i^* + \delta K_i^*)$ are zero according to Eq. (5), it implies that

$$\sum_{i=1}^{i=n} \delta U_i^* = 0. \quad (19)$$

The energy invariance

$$E^* = U_n^*(\mathbf{R}_n) + K_n^*(\mathbf{R}_{n-1}, \mathbf{R}_n) \quad (20)$$

is given by the start condition for the discrete dynamics and it differs from the energy invariance of Newtonian dynamics. It is a state function, and due to the discrete dynamics it depends on two consecutive sets of the positions, $\mathbf{R}_{n-1}$, $\mathbf{R}_n$, instead of the energy invariance in Newtonian dynamics which depends on the positions $\mathbf{R}(t_n)$ and the momenta $\mathbf{P}(t_n)$ at the same time t_n. The two invariances are, however, equal in the analytic limit[10]

$$\lim_{h\to 0}\left(\delta U_n^* + \delta K_n^*\right) = -\mathbf{F}(t_n)\cdot\delta\mathbf{R}(t_n) + \delta K(t_n) + \mathcal{O}(h^2) = 0, \quad (21)$$

where the term $\mathcal{O}(h^2) = \frac{h^2}{2}\mathbf{F}(t_n)^2$ is the *total deviation* from the Newtonian dynamics.

The invariance, Eq. (20) does not depend on a convergence of an asymptotic expansion, and it differs also from the shadow energy for the shadow Hamiltonian by that, although the change contains two terms, the expressions for their changes do not make use of a potential, but only of the forces and the discrete positions. It is obtained by noticing that, with a suitable definition of the "work" and kinetic energy, $\delta U_n^* = -\delta K_n^*$, and by formulating the requirement that $U_n^*(\mathbf{R}_n)$ is a state function. The derivation is a copy of the derivation of the energy invariance for Newtonian dynamics.[10] In Thermodynamics, the First law of thermodynamics is formulated exactly in the same manner, but as a basic assumption of that the energy function is a state function consisting of two terms which change by work and kinetic energy exchanges, and the present formulations is the corresponding formulation of the energy conservation in dynamics and thermodynamics for discrete VA dynamics.

A. Energy conservation in MD with VA dynamics

The formulation of energy in discrete VA dynamics by the ability $U^*(\mathbf{R})$ to perform a discrete work instead of the potential energy $U(\mathbf{R})$ works equally well as the traditional formulation. Molecular Dynamics simulations with VA for N particles are obtained from two consecutive start sets of positions, $\mathbf{R}_0$ and $\mathbf{R}_1$, and these positions define not only the total dynamics evolution, but also the mean value of traditional zero order energy, $\langle E(0)_n\rangle$, the accurate first order estimate of the shadow energy, $\tilde{E}_n \approx E(0)_n + h^2E(1)_n$ of the underlying analytic dynamics and the exact energy invariance E^*. Since the change in E^* is given in the same manner as the energy conservation by the First law of thermodynamics, we need to define a "start ability," U_1^* for the discrete dynamics. But the discrete VA dynamics differs in fact neither from the analytic counterpart at this point. In principle, we could obtain the ability U_1^* at the start of the simulation by determining the discrete work performed by bringing the particles from infinite separations via $\mathbf{R}_0$ to the positions $\mathbf{R}_1$. In the thermodynamics one defines, however, a standard state of energy (enthalpy), and here we will use the potential energy $U_1(\mathbf{R}_1)$ at the positions $\mathbf{R}_1$ and the accurate estimate, $\tilde{E}_1$ at the start of the dynamics, and obtain

$$U_1^* = U_1(\mathbf{R}_1) \quad (22)$$

and the energy invariance

$$E^*(t_{n+1}) = \tilde{E}_1 + \sum_{i=1}^{i=n}[\delta U_n^* + \delta K_n^*] \quad (23)$$

with

$$\delta U_n^* = -\mathbf{F}_i\cdot(\mathbf{R}_{i+1}-\mathbf{R}_i) + \frac{h^2}{2}\mathbf{F}_i^2. \quad (24)$$

The energy evolution by MD in double precision arithmetic with VA was determined for two systems. In the first a liquid system of $N = 2000$ LJ particles at the density $\rho = 0.80\sigma^3$ was calibrated at the temperature $kT/\epsilon = 1$. The thermostat[8] was switched off and the energy evolution in the next 10 000 time steps with $h = 0.005$ was obtained.

Figure 1 shows the energy evolution $E(0)_n$, $\tilde{E}_n$, and E_n^* for the first 100 time steps. The first order estimate of $\tilde{E}_n$ (green dashes) improves the accuracy of the energy determination with a factor of hundred, the energy invariance E^* is exact (see inset).

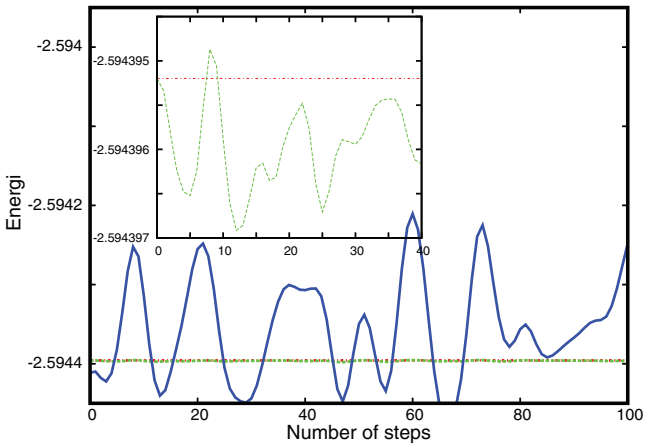

FIG. 1. Discrete energies of a LJ system with the Verlet algorithm at T, $\rho = 1.0$, 0.80, and for $h = 0.005$. Blue solid line: traditional energy estimate $E(0)_n$; green dashed line: "shadow" energy $\tilde{E}_n \approx E(0)_n + h^2E(1)_n$; red dashed-dotted line: the energy invariance E^*. The inset shows $\tilde{E}_n$ and E^*.

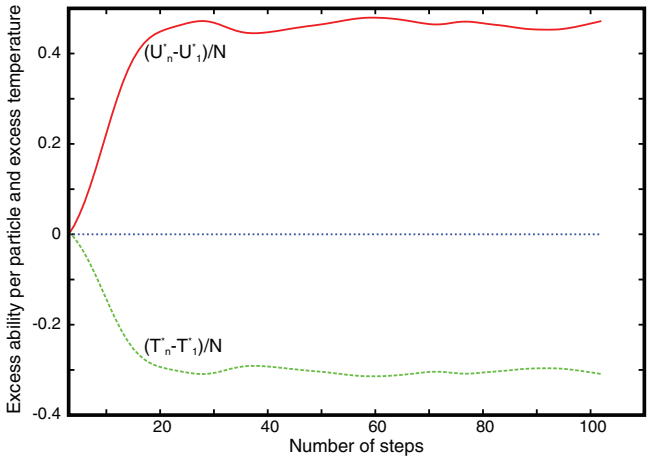

FIG. 2. Excess discrete energies end temperatures of a non-equilibrium system of $N = 2048$ LJ particles at spontaneous melting . Red line: the excess ability per particle $(U_n^* - U_1^*)/N$; green long dashed line: excess temperature $T_n^* - T_1^*$; blue short dashed line: the constant energy invariance $E_n^* = E_1^*$.

The constant VA dynamics is obtained from two sets of positions, $\mathbf{R}_0$, $\mathbf{R}_1$ and h and these start values cannot contain information about whether the system is in equilibrium or not. In order to obtain the evolution of the kinetic energy K_n^* and the ability U_n^* in a non-equilibrium system with VA dynamics a system was started with two sets of positions which correspond to a non-equilibrium state. The non-equilibrium state was obtained for a system of $N = 2048$ LJ particles in a fcc solid at $kT/\epsilon = 1$ and density $\rho = 1.009\sigma^3$ (density of coexisting solid at $kT/\epsilon = 1$[11]) by spontaneously expanding the positions to the density $\rho = 0.80\sigma^3$ by a scaling of all the positions $\mathbf{R}_0$, $\mathbf{R}_1$. A LJ systems equilibrium state at the density $\rho = 0.80\sigma^3$ is a liquid. The fcc ordered system melted spontaneously, and the conservative systems temperature decreased according to the Second law of Thermodynamics. The change in the temperature at the spontaneous melting is shown with green dashes in Figure 2. The temperature decreased from $T_1^* = 1$ within 20–40 time steps to $T^* \approx 0.7$. The differences between T_n^* and the temperature $\tilde{T}_n$, obtained for the shadow Hamiltonian,[8] are of the order 10^{-7}, and they are not visible in the figure. The decrease in the spontaneous temperature at the melting was balanced by a corresponding increase in the ability (red line), and the energy invariance E^* (blue small dashes) was constant in the conservative system. The two MD simulations (Figures 1 and 2) demonstrate that the traditional and the present (discrete) energy concept work equally well.

III. DISCRETE DYNAMICS VERSUS ANALYTIC DYNAMICS

The discrete VA dynamics has the same invariances as Newtonian dynamics and it raises the question: Which of these formulations that are correct, or alternatively, the most appropriate formulation of classical dynamics? In this context Lee in 1983 wrote a paper[12] entitled, "Can Time Be a Discrete Dynamical Variable?"; which led to a series of publications by Lee and co-workers on the formulation of fundamental dynamics in terms of difference equations, but with exact invariance under continuous groups of translational and rotational transformations. Quoting Lee,[13] he "wish to explore an alternative point of view: that physics should be formulated in terms of difference equations and that these difference equations could exhibit all the desirable symmetry properties and conservation laws." Lee's analysis covers not only classical mechanics,[12] but also non relativistic quantum mechanics and relativistic quantum field theory,[14] and Gauge theory and Lattice Gravity.[13] The discrete dynamics is obtained by treating positions and time, *but not momenta*, as a discrete dynamical variables, and he obtained a conserved (mean) "energy" over consecutive time intervals of different lengths. But according to Lee[12] in his formulation of discrete mechanics, "there is a *fundamental length* or time l (in natural units). Given any time interval $T = t_f - t_0$, the total number N of discrete points that define the trajectory is given by the integer nearest T/l."

The analogy between Lee's formulation of discrete dynamics and VA dynamics is striking. For the VA dynamics one uses a *unit time increment, h*, and the momenta are not dynamical variables and they have no impact on the discrete dynamics.[2] The fundamental length and time in quantum electrodynamics are the Planck length $l_P \approx 1.6 \times 10^{-35}$ m and Planck time $t_P \approx 5.4 \times 10^{-44}$ s,[15] and they are immensely smaller than the length unit (given by the floating point precision) and time increment used in MD to generate the classical discrete dynamics. But the analogy implies that the discrete VA dynamics obtained by MD is the "continuation" of the Lee's discrete quantum dynamics for a fundamental length of time t_P, as is the analytic classical dynamics of the traditional quantum mechanics, given by the Wigner expansion.[16]

The discrete non relativistic quantum mechanics is obtained by Lee using Feynman's path integration formalism, but for discrete positions and a corresponding discrete action,

$$\mathcal{A}_D = \sum_{n=1}^{N+1} \left[\frac{(\mathbf{R}_n - \mathbf{R}_{n-1})^2}{2(t_n - t_{n-1})} + (t_n - t_{n-1})\overline{V(n)} \right], \qquad (25)$$

where $\mathbf{R}_{N+1}$ is the end-positions at time t_{N+1} and the minimum of $\mathcal{A}_D$ determines the classical path. The action is a sum over products of time increments and "kinetic energies" K_n^*, and Lee has used the symbol $\overline{V(n)}$, for the average of "potential energy" in the time intervals $[t_{n-1}, t_n]$. The momenta for all the paths, given by the discrete nodes $\mathbf{R}_1$, .., $\mathbf{R}_{N+1}$, are obtained from differences, $\mathbf{R}_n - \mathbf{R}_{n-1}$, so the classical VA discrete trajectory is the classical limit path for discrete quantum mechanics with $h = t_P$, as the classical Newtonian trajectory is for the traditional quantum mechanics. There is, however, one important difference between the analytic and the discrete dynamics. The momenta *for all the paths* in the discrete quantum dynamics are obtained by a difference between discrete sets of positions and they are all *asynchronous* with the positions. So the Heisenberg uncertainty is a trivial consequence of a discrete quantum electrodynamics with a fundamental length of time t_P.

Lee motivates his reformulation of the analytic dynamics in the Introduction in Ref. 14 by the difficulties of formulating a general *unifying* theoretical model for dynamics and with the Concluding Remarks in Ref. 13 that (he tries to explore

the opposite viewpoint): "Difference equations are more fundamental, and differential equations are regarded as approximations." The difference in the energy between the analytic energy and the energy obtained by Eq. (21) for discrete electrodynamics with a unit time increment t_P is of the order t_P^2, and it is absolute marginal. The Heisenberg uncertainty between positions and momenta is of the order t_P and this uncertainty is an inherent quality of discrete dynamics with a fundamental length of time t_P. The discrete classical VA dynamics is fundamentally different from analytic Newtonian dynamics, but has the same invariances and the dynamics is obtained equally well by both methods. But, on the other hand the traditional quantum mechanics is in all manner fully appropriate and justifies no revision of the formulation, and an eventual revision of the dynamics must be justified by other facts than conservation of the energy by classical Molecular Dynamics simulation with the VA algorithm.

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