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## Principles of discrete time mechanics: I. Particle systems

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**Abstract.** We discuss the principles to be used in the construction of discrete time classical and quantum mechanics as applied to point particle systems. In the classical theory this includes the concept of virtual path and the construction of system functions from classical Lagrangians, Cadzow's variational principle applied to the action sum, Maeda–Noether and Logan invariants of motion, elliptic and hyperbolic harmonic oscillator behaviour, gauge invariant electrodynamics and charge conservation, and the Grassmannian oscillator. First quantized discrete time mechanics is discussed via the concept of system amplitude, which permits the construction of all quantities of interest such as commutators and scattering amplitudes. We discuss stroboscopic quantum mechanics, or the construction of discrete time quantum theory from continuous time quantum theory and show how this works in detail for the free Newtonian particle. We conclude by applying the Schwinger action principle to the important case of the quantized discrete time inhomogeneous oscillator.

### 1. Introduction

There are various circumstances in mechanics where it is convenient or necessary to replace the continuous time (temporal evolution) parameter with a discrete parameter. Computer simulation of waves is an example where the configuration of a system at time  $t + T$  is calculated from a knowledge of its configuration at times  $t$  and  $t - T$ . There have been various attempts to construct classical and quantum mechanical theories based on this notion, such as the work of Cadzow [1], Logan [2], Maeda [3] and Lee [4]. The work of Yamamoto *et al* [5], Hashimoto *et al* [6] and Klimek [7] indicates that the subject continues to receive attention.

This paper considers the question: by which principles if any should continuous time mechanical theories be discretized, that is, turned into discrete time analogues? By discretization we do not mean the numerical approximation of continuous time mechanics such as the work of Bender *et al* [8]. Neither do we discretize space or the dynamical degrees of freedom. Our attention is fixed solely on replacing a continuous dynamical evolution parameter with a discrete parameter. In this and the following paper, paper II on discrete time classical field theory [9], our interest is in the construction of exact, self-consistent discrete time mechanics with well specified principles, equations of motion and predictions. This is motivated by the notion that at some unimaginably small scale, time is really discrete. This has echoes in modern theories such as string theory and quantum gravity, where the Planck time of  $10^{-43}$  seconds sets a scale at which conventional notions of space and time break down.

It could be argued that relativity requires a symmetrical treatment between time and space but this leads to the situation of a spacetime lattice approach which has lost all

relativistic symmetries and rotational invariance. We argue that relativity does distinguish between timelike and spacelike, and by discretizing only time our approach reduces the break with relativity to a minimum. Lorentz covariance is broken in our approach to field theories, discussed in paper II, but the residual Euclidean invariances permit the construct of particle-like states.

It may be felt objectionable that there is no natural concept of velocity in discrete time mechanics. It could be argued that this lack destroys our intuitive feeling for dynamics based on the notion of (say) a particle system evolving from an initial position and an initial velocity. The correct way to see the situation is in terms of real numbers. In continuous time mechanics, we normally consider a particle as having an instantaneous position and an instantaneous velocity (we exclude Brownian particle dynamics from our definition of continuous time mechanics). This information requires two real numbers for every degree of freedom. In discrete time mechanics, there is no natural concept of simultaneity analogous to this. What we mean by a ‘particle’ is something with a position at time  $t$  and a position at time  $t - T$ , which also requires two real numbers for every degree of freedom. A particle here is more properly associated with the *link* between two successive points in discrete time, rather than those times separately. So ultimately, the only major difference in principle between continuous time and discrete time mechanics is the lack of the limit process  $T \rightarrow 0$ .

One problem with discrete time mechanics is a lack of guiding principles at key places, which our series of papers attempts to address. For example, consider the discretization of a system with Lagrangian  $L = \frac{1}{2}m\dot{x}^2 - V(x)$ . The approach taken by most authors would be to replace the temporal derivatives by differences, symmetrize the potential in some way, derive the analogue of the Euler–Lagrange equation, and finally evolve the system according to the resulting difference equation. Quantities such as the energy  $E = \frac{1}{2}m\dot{x}^2 + V(x)$  which are conserved in continuous time mechanics would be monitored by calculating the value  $E_D$  of the discretized Hamiltonian.

It is more than likely however that a naive discretization of the Hamiltonian would result in an expression  $E'_D$  which is not exactly conserved. This has been discovered by many authors. It is a particular merit of Lee’s approach [4] that an invariant analogous to the energy drops out of the formalism, but only at the expense of a dynamically evolving discrete time interval.

It is somewhat surprising therefore that a computer simulation based on the above principles should be judged as good or bad according to how constant  $E'_D$  remains. In the absence of any proper principle for the construction of invariants of motion it should come as no surprise to find that occasionally a quantity such as  $E'_D$  will vary enormously and unpredictably during the course of a simulation. This happens because there are actually three systems being confused; (1) the original continuous time theory, (2) a discrete time system evolving exactly according to some well defined discretized Euler–Lagrange equation, and (3) some unknown discrete time system for which the naively discretized energy,  $E'_D$ , would be an exact constant of the motion, but only for evolution under its own discretized equation of motion, which could be very different to the equation of motion for (2). On top of this there may be numerical uncertainties induced by the computer algorithms used. Seen in this light, it would seem a wise policy to discretize according to definite principles which would establish conserved quantities rigorously. The construction of invariants of motion therefore becomes one of the principal objectives of discrete time mechanics.

An important first step in the process of constructing rigorous discrete time mechanics was the introduction of a discrete time action principle. This was done by Cadzow [1],

giving a discrete time analogue of the Euler–Lagrange equation. We shall call such an equation a *Cadzow’s equation* for the system. The construction of constants of motion was considered by Maeda [3] in the case of continuous symmetries, whilst the construction of constants of motion analogous to the energy had previously been considered by Logan [2].

Various features found in continuous time mechanics have discrete time analogues, including Noether’s theorem, whilst certain other features either do not or cannot have discrete time analogues. A particular problem arises, for example, with Hamiltonian evolution and equations of motion derived using Poisson brackets. Not only is there no possibility here of an infinitesimal translation in time (which thereby renders the notion of a Hamiltonian problematic) but there is no natural concept of velocity as a limit either. This makes the standard definition of conjugate momentum as the partial derivative of the Lagrangian with respect to a velocity just as problematic. This has not prevented a number of authors from constructing discrete time analogues of Poisson brackets, however, with various degrees of success and utility, usually with the observation that the generator of time translations is not conserved.

A feature of our approach is that we have found a clear principle for the definition of conjugate momentum in discrete time mechanics. It turns out *not* to be the partial derivative of the ‘Lagrangian’ with respect to a difference in general, but does reduce to it in various important cases. In addition, we have avoided trying to construct Hamiltonians and equations of motion derived via Poisson brackets. In our formalism the Hamiltonian is displaced by a Logan invariant, if such a quantity can be found. Fortunately such an object does exist for the important case of the harmonic oscillator, which has ramifications in the discrete time field theory discussed in the next paper in this series.

The overall plan for this and subsequent papers is as follows. In this paper (paper I) we restrict our attention to classical and quantum point particle dynamics, reserving classical field theory to paper II, quantum field theory to paper III, and quantum electrodynamics to paper IV.

Topics covered in paper I are as follows. First we introduce the central concept of *system function*. This replaces the Lagrangian as the key to the dynamics. With the system function we can calculate equations of motion, construct invariants of the motion, and quantize the system. We give a prescription for constructing the system function from a given Lagrangian. We may use this prescription to embed symmetries into the system function such as gauge invariance and hence construct electrodynamics. Then we discuss the construction of invariants based on the work of Maeda, Noether, and Logan, and apply it to the harmonic oscillator, which we discuss in detail. This key system lies at the heart of particle field theory, discussed in the following papers, and it displays some important properties, such as a natural cut-off for particle energy, for example. We also discuss particle electrodynamics and the Grassmannian oscillator.

A major part of our programme is to develop discrete time quantum mechanics and so we conclude our paper with a discussion of the principles for first quantization. This includes the concept of system amplitude, the construction of unequal-time commutators, and compatible operators. We then discuss the construction of discrete time quantum mechanics from standard quantum mechanics via a stroboscopic approach and give an explicit example. Finally, we apply the Schwinger action principle to the discrete time inhomogeneous harmonic oscillator to construct the Feynman propagator for the oscillator, in anticipation of its use in field theory.

## 2. Action integrals and action sums

In continuous time mechanics Lagrangian dynamics is conventionally formulated via an action principle based on the action integral

$$A_{if}[\Gamma] = \int_{t_i}^{t_f} dt L(\mathbf{q}, \dot{\mathbf{q}}, t) \quad (1)$$

where  $t_i$  and  $t_f$  are the initial and final times respectively along some given path  $\Gamma$ . In our version of discrete time mechanics we postulate that the dynamical variables  $\mathbf{q}(t)$  are observed or sampled at a finite number of times  $t_n, n = 0, 1, \dots, N$ , where  $t_0 = t_i$  and  $t_N = t_f$ , such that the intervals  $t_{n+1} - t_n$  are all equal to some fundamental interval  $T$ . For convenience we will write  $\mathbf{q}_n \equiv \mathbf{q}(t_n)$ .

It is possible to develop a theory where the time intervals vary dynamically along the path. Such a mechanics was considered by Lee [4]. The extension of our methods to that particular situation is left for a further article.

In our formulation of discrete time mechanics we replace the action integral (1) by an action sum of the form

$$A^N[\Gamma] = \sum_{n=0}^{N-1} F^n \quad (2)$$

where  $F^n \equiv F(\mathbf{q}_n, \mathbf{q}_{n+1}, n)$  will be referred to as the *system function*. The system function has the same central role in discrete time mechanics as the Lagrangian has in continuous time mechanics. With it we may construct the equations of motion, define conjugate momenta, construct constants of motion and attempt to quantize the system. In principle, we could consider higher-order system functions which depend on (say)  $\mathbf{q}_n, \mathbf{q}_{n+1}, \dots, \mathbf{q}_{n+r}, r \geq 2$ , but the case  $r = 1$  represents the simplest possibility which could give rise to non-trivial dynamics and will be considered exclusively from now on. Such system functions are the discrete time analogues of Lagrangians of the canonical form  $L = L(\mathbf{q}, \dot{\mathbf{q}}, t)$ .

Another reason for considering only a second-order formulation ( $r = 1$ ) is its direct relationship to Hamilton's principal function, discussed presently. Cadzow [1] applied a variational principle to an action sum such as (2) and derived the equation of motion

$$\frac{\partial}{\partial \mathbf{q}_n} \{F^{n-1} + F^n\}_c = \mathbf{0} \quad 0 < n < N \quad (3)$$

where the symbol  $\frac{\partial}{\partial \mathbf{q}_n} \{ \}_c$  denotes an equality holding over a true or dynamical trajectory. We shall refer to (3) as a *Cadzow's equation of motion* for the system. We now discuss the interpretation of this equation.

Suppose we have a continuous time action integral of the form (1). First, partition the time interval  $[t_0, t_N]$  into  $N$  equal subintervals. Then the action integral may be written as a sum of subintegrals, i.e.

$$A_{if}[\Gamma] = \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} dt L(\mathbf{q}(t), \dot{\mathbf{q}}(t), t). \quad (4)$$

Now suppose that we fixed the coordinates  $\mathbf{q}_n$  at the various times  $t_0, t_1, \dots, t_N$  and then choose the path connecting each pair of points  $(\mathbf{q}_n, \mathbf{q}_{n+1})$  to be the true or dynamical path, that is, a solution to the Euler–Lagrange equations of motion for those boundary conditions. If this partially extremized path is denoted by  $\tilde{\Gamma}_c$  then we may write

$$A_{if}[\tilde{\Gamma}_c] = \sum_{n=0}^{N-1} S^n \quad (5)$$

where  $S^n \equiv S(\mathbf{q}_{n+1}, t_{n+1}; \mathbf{q}_n, t_n)$  is known as Hamilton's principal function, being just the integral of the Lagrangian along the true path from  $\mathbf{q}_n$  at time  $t_n$  to  $\mathbf{q}_{n+1}$  at time  $t_{n+1}$ .

We recall now that the canonical momenta  $\mathbf{p}_n^{(+)}$ ,  $\mathbf{p}_{n+1}^{(-)}$  at the endpoints  $\mathbf{q}_n$ ,  $\mathbf{q}_{n+1}$  may be obtained from Hamilton's principal function via the rule

$$\mathbf{p}_{n+1}^{(-)} \equiv \frac{\partial}{\partial \mathbf{q}_{n+1}} S^n \quad \mathbf{p}_n^{(+)} \equiv -\frac{\partial}{\partial \mathbf{q}_n} S^n \quad (6)$$

where the superscript (+) denotes that the momentum at the initial time,  $t_i$ , carries information *forwards*, whereas the superscript (−) denotes that the momentum at the final time,  $t_f$ , is influenced by earlier dynamics with respect to the temporal interval concerned. At this stage the action sum (5) has not been extremized fully, as the intermediate points  $\mathbf{q}_n$ ,  $0 < n < N$  have been held fixed.

Now suppose we went further and extremized (5) fully by variation of the previously fixed intermediate coordinates  $\mathbf{q}_n$ ,  $n = 1, 2, \dots, N - 1$ . Then we would find that

$$\frac{\partial}{\partial \mathbf{q}_n} \{S^{n-1} + S^n\}_c = \mathbf{0} \quad 0 < n < N. \quad (7)$$

This equation may be understood as the condition that the canonical momentum along the true path from  $\mathbf{q}_i$  to  $\mathbf{q}_f$  is continuous, that is,  $\mathbf{p}_n^{(+)} = \mathbf{p}_n^{(-)}$ . We notice immediately that (7) has the same formal structure as Cadzow's equation (3) provided we make the identification  $F^n \leftrightarrow S^n$ .

Another interpretation of Cadzow's equation is that it endows the action sum with the additivity property of action integrals, which satisfy the relations

$$\int_{t_0}^{t_1} dt L + \int_{t_1}^{t_2} dt L = \int_{t_0}^{t_2} dt L \quad t_0 < t_1 < t_2. \quad (8)$$

This property holds for all trajectories in continuous time mechanics, and not just for the true or classical trajectory. In the case of system functions we may write

$$F(\mathbf{q}_{n-1}, \mathbf{q}_n) + F(\mathbf{q}_n, \mathbf{q}_{n+1}) = f(\mathbf{q}_{n-1}, \mathbf{q}_{n+1}) \quad (9)$$

for some function  $f$  of  $\mathbf{q}_{n-1}$  and  $\mathbf{q}_{n+1}$ , because Cadzow's equation (3) is equivalent to the statement that  $F^n + F^{n-1}$  is independent of  $\mathbf{q}_n$  along dynamical trajectories. However, unlike action integrals, this property will not hold off the true or classical trajectory in general.

### 3. System functions from Lagrangians

Two important ideas emerge from the similarity between (3) and (7).

(i) Although the concept of velocity as a limit does not occur in discrete time mechanics, we will define a unique discrete time momentum,  $\mathbf{p}_n$ , conjugate to  $\mathbf{q}_n$  by the rule

$$\mathbf{p}_n \equiv -\frac{\partial}{\partial \mathbf{q}_n} F^n. \quad (10)$$

This should be compared with the approach of Yamamoto *et al* [5] and Hashimoto *et al* [6] and most other workers, where the momentum is defined as a derivative of a discretized Lagrangian with respect to a difference. In our terms Cadzow's equation reduces simply to the statement that we may also calculate this momentum via the rule

$$\mathbf{p}_n \equiv \frac{\partial}{\partial \mathbf{q}_n} F^{n-1}. \quad (11)$$

(ii) We will construct a system function  $F^n$  from the temporal integral from  $t_n$  to  $t_{n+1}$  of a continuous time Lagrangian, the question being which path to take. We cannot in general consider using the true continuous time path, as this is meaningless in the context of discrete time mechanics and normally not known to us. For the particularly important case of the harmonic oscillator, however, we can evaluate Hamilton's principal function precisely and this provides us with an important check on our formalism. The path chosen in the construction of the system function will be referred to as a *virtual path*.

It is possible to choose from a number of possible virtual paths, such as those inspired by  $q$ -deformed mechanics [7]. This does not alter any of the principles we employ, it simply changes the details of the system function used and hence the sort of invariants of motion we can find. In this paper we are interested in treating time homogeneously, and so we choose a temporal lattice with a constant fundamental time interval  $T$ . Our proposed solution for the virtual path in point particle mechanics is to take the geodesic or shortest geometric path from  $\mathbf{q}_n$  to  $\mathbf{q}_{n+1}$ , the metric normally being the Euclidean one in physical space (not in coordinate space). This prescription will normally provide us with a unique system function from a given Lagrangian. Moreover, it should be applicable to configuration spaces with curvature and is a coordinate frame independent concept. It allows us to construct a gauge-invariant discrete time prescription for electrodynamics, with a suitable modification. In paper II of this series we shall show that we can also apply this prescription successfully to field theories. There may be important cases where the chosen virtual path is not a linear interpolation. This occurs for charged fields in the next paper in the series. In such cases, additional requirements such as gauge invariance will influence the choice of virtual path.

To illustrate the procedure, consider a non-relativistic particle with position vector  $\mathbf{x}$  and Lagrangian  $L(\mathbf{x}, \dot{\mathbf{x}}, t)$ . Then the virtual path  $\tilde{\mathbf{x}}_n$  taken between  $\mathbf{x}_n$  and  $\mathbf{x}_{n+1}$  is given by

$$\tilde{\mathbf{x}}_n = \lambda \mathbf{x}_{n+1} + \bar{\lambda} \mathbf{x}_n \quad (12)$$

where  $0 \leq \lambda \leq 1$  and  $\bar{\lambda} \equiv 1 - \lambda$ . With this choice of virtual path the time derivative becomes a difference operator. Specifically, we find

$$\tilde{\mathbf{v}}_n \equiv \frac{d}{d\tilde{t}} \tilde{\mathbf{x}}_n = \frac{\mathbf{x}_{n+1} - \mathbf{x}_n}{T} \quad (13)$$

where we define

$$\tilde{t}_n \equiv \lambda t_{n+1} + \bar{\lambda} t_n = t_n + \lambda T. \quad (14)$$

Then we construct the system function via the rule

$$F^n \equiv T \int_0^1 d\lambda L(\tilde{\mathbf{x}}_n, \tilde{\mathbf{v}}_n, \tilde{t}_n). \quad (15)$$

The use of this integration does not imply that continuous time is regarded as being meaningful in the context of discrete time mechanics. We are interested only in the results, not in the means of obtaining these results. A useful analogy is with the use of classical mechanics to set up quantum mechanical models. Once we have found our quantum theory, we no longer need to regard the classical model which generated it as any more than some approximation useful in some circumstances. Our prescription allows us to embed into our system function fundamental properties such as gauge invariance and other symmetries of importance to physics.

If the Lagrangian is a real analytic function of its arguments then we may make a Taylor expansion about  $\mathbf{x}_n$  and integrate term by term. This will be valid for Lagrangians which

are polynomial functions of  $\mathbf{x}$  and  $\dot{\mathbf{x}}$ . In such cases the system function  $F^n$  would be given by the formal expression

$$F^n = T \sum_{m=0}^{\infty} \frac{T^m (D_n)^m}{(m+1)!} L(\mathbf{x}_n, \mathbf{v}_n, t_n) \quad (16)$$

where  $D_n$  is the operator  $\mathbf{v}_n \cdot \frac{\partial}{\partial \mathbf{x}_n} + \frac{\partial}{\partial t_n}$  and  $\mathbf{v}_n$  and  $\mathbf{x}_n$  are considered independent at this stage.

Some examples will illustrate the process. For a particle in one dimension with Lagrangian

$$L = \frac{1}{2} m \dot{x}^2 - \sum_{r=0}^{\infty} C_r x^r \quad (17)$$

where the  $C_r$  are constants, the system function is given formally by

$$F^n = \frac{m(x_{n+1} - x_n)^2}{2T} - T \sum_{r=0}^{\infty} \frac{C_r (x_{n+1}^{r+1} - x_n^{r+1})}{(r+1)(x_{n+1} - x_n)}. \quad (18)$$

For instance, the anharmonic oscillator Lagrangian

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 - \frac{1}{4} m \lambda x^4 \quad (19)$$

gives the system function

$$F^n = \frac{m(x_{n+1} - x_n)^2}{2T} - \frac{T m \omega^2 (x_{n+1}^3 - x_n^3)}{6(x_{n+1} - x_n)} - \frac{T m \lambda (x_{n+1}^5 - x_n^5)}{20(x_{n+1} - x_n)}. \quad (20)$$

This differs from the anharmonic oscillator system function discussed in [10, 11], which illustrates the general problem with discrete time mechanics. There may be many possible discretizations of a given continuous time system, all of which lead back to the continuous time theory when we take appropriate limits. The principle specified above gives us a unique discretization (subject to choice of virtual path).

For the Coulombic potential problem in three spatial dimensions, the Lagrangian

$$L = \frac{m}{2} \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + \frac{\gamma}{|\mathbf{x}|} \quad (21)$$

with virtual path (12) gives the system function

$$F^n = \frac{m(\mathbf{x}_{n+1} - \mathbf{x}_n)^2}{2T} + \frac{\gamma T}{|\mathbf{x}_{n+1} - \mathbf{x}_n|} \ln \left\{ \frac{\mathbf{x}_{n+1} \cdot (\mathbf{x}_{n+1} - \mathbf{x}_n) + |\mathbf{x}_{n+1}| |\mathbf{x}_{n+1} - \mathbf{x}_n|}{\mathbf{x}_n \cdot (\mathbf{x}_{n+1} - \mathbf{x}_n) + |\mathbf{x}_n| |\mathbf{x}_{n+1} - \mathbf{x}_n|} \right\}. \quad (22)$$

This system function leads to Cadzow's equations of motion which preserve the discrete time analogue of orbital angular momentum. This system function is markedly different in form to the original Coulombic Lagrangian (21) but if we consider trajectories for which we may write  $\mathbf{x}_n \equiv \mathbf{r}_n$ ,  $\mathbf{x}_{n+1} \equiv \mathbf{r}_n + T \mathbf{v}_n + O(T^2)$  for each  $n$ , then

$$\lim_{T \rightarrow 0} \left\{ \frac{F_n}{T} \right\} = \frac{1}{2} m \mathbf{v}_n \cdot \mathbf{v}_n + \frac{\gamma}{|\mathbf{r}_n|} \quad (23)$$

which corresponds with (21). However, it should be kept in mind that there will be many discrete time trajectories for which this limit cannot be taken. For example, there may be trajectories where the particle repeatedly flips between two fixed positions only. This may happen with the discrete time harmonic oscillator, for example, and no limit such as the one discussed above exists for such a trajectory. Discrete time mechanics is inherently richer in its set of possible trajectories than continuous time mechanics.



In general, Cadzow's equations lead to an implicit equation for  $x_{n+1}$  involving  $x_n$  and  $x_{n-1}$ , although for certain systems such as the harmonic oscillator discussed below we may solve Cadzow's equation to find  $x_{n+1}$  explicitly. The situation is analogous to what happens in computer simulations of partial differential equations where not all equations give  $x_{n+1}$  explicitly. In such cases we must use numerical techniques to solve for the  $x_{n+1}$  in the classical theory. It is a special feature of our approach that our equations of motion involve only  $x_{n-1}$ ,  $x_n$ , and  $x_{n+1}$ , which is not always the case with finite difference schemes used to approximate differential equations.

#### 4. Invariants of motion

It is possible to find a discrete time analogue of Noether's theorem in the case of continuous symmetries along the lines considered by Maeda [3]. We shall refer to constants of motion found by this theorem as *Maeda–Noether invariants*. Consider a system function  $F^n \equiv F(\mathbf{q}_n, \mathbf{q}_{n+1})$  which is invariant to some point transformation  $\mathbf{q}_n \rightarrow \mathbf{q}'_n = \mathbf{q}_n + \delta\mathbf{q}_n$ . Then we may write

$$\begin{aligned} 0 = \delta F^n &= \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \delta \mathbf{q}_n + \frac{\partial F^n}{\partial \mathbf{q}_{n+1}} \cdot \delta \mathbf{q}_{n+1} \\ &= \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \delta \mathbf{q}_n - \frac{\partial F^{n+1}}{\partial \mathbf{q}_{n+1}} \cdot \delta \mathbf{q}_{n+1} \end{aligned} \quad (24)$$

using Cadzow's equation of motion. From this we deduce that the quantity  $C^n \equiv \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \delta \mathbf{q}_n$  will be conserved along dynamical trajectories, that is,

$$C^n = C^{n+1}. \quad (25)$$

This construction does not allow us to construct an analogue of the Hamiltonian in the case of conserved systems because in our formulation we are not allowed to make infinitesimal jumps in time.

Logan [2] gave a method for constructing constants of motion which are not necessarily related to symmetries of the system function. Consider a point transformation

$$\mathbf{q}_n \rightarrow \mathbf{q}'_n = \mathbf{q}_n + \epsilon \mathbf{u}_n \quad (26)$$

where  $\epsilon$  is infinitesimal and  $\mathbf{u}_n$  is a function of  $\mathbf{q}_n$  and  $\mathbf{q}_{n+1}$ . Then

$$\delta F^n = \epsilon \left\{ \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \mathbf{u}_n + \frac{\partial F^n}{\partial \mathbf{q}_{n+1}} \cdot \mathbf{u}_{n+1} \right\} = \epsilon \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \mathbf{u}_n - \epsilon \frac{\partial F^{n+1}}{\partial \mathbf{q}_{n+1}} \cdot \mathbf{u}_{n+1} \quad (27)$$

on the true trajectories. Now suppose that transformation (26) is such that  $\delta F^n$  can be written in the form  $\delta F^n = \epsilon v_{n+1} - \epsilon v_n$ , where  $v_n = v(\mathbf{q}_n)$ . Then we immediately deduce that the quantity

$$C^n \equiv \frac{\partial F^n}{\partial \mathbf{q}_n} \cdot \mathbf{u}_n + v_n \quad (28)$$

is conserved over the classical trajectories. Such a constant of motion will be referred to as a *Logan invariant*.

## 5. The discrete time harmonic oscillator

### 5.1. A Logan invariant for the harmonic oscillator

The discrete time harmonic oscillator in its generic form is given by the quadratic system function

$$F^n = \frac{1}{2}\alpha(x_n^2 + x_{n+1}^2) - \beta x_n x_{n+1} \quad \beta \neq 0 \quad (29)$$

which gives Cadzow's equation of motion

$$x_{n+1} = \frac{c}{2\eta} x_n - x_{n-1} \quad \eta = \frac{\alpha}{\beta}. \quad (30)$$

A Logan invariant of motion is found to be

$$C^n \equiv \frac{1}{2}\beta(x_n^2 + x_{n+1}^2) - \alpha x_n x_{n+1}. \quad (31)$$

### 5.2. Limiting behaviour

In this section we show how to solve the equation of motion (30) and determine the behaviour of the oscillator as the discrete time tends to infinity. First we define the variables

$$a_n^\pm \equiv x_n - \mu^\pm x_{n+1} \quad (32)$$

which will become the analogues of annihilation and creation operators in quantum theory. The constants  $\mu^\pm$  are chosen to satisfy the condition

$$a_n^\pm = \mu^\pm a_{n-1}^\pm \quad (33)$$

under the equation of motion (30), which implies

$$a_n^\pm = (\mu^\pm)^n a_0^\pm. \quad (34)$$

Condition (33) gives

$$\mu^\pm = \eta \pm \sqrt{\eta^2 - 1}. \quad (35)$$

We note that  $\mu^+ \mu^- = 1$ . The Logan invariant (31) is given by

$$C^n = \frac{1}{2}\beta a_n^+ a_n^- \quad (36)$$

which is a constant of motion by inspection and is a form of great value in discrete time field theory.

The complete solution to the problem is now readily obtained and given by

$$x_n = \frac{c}{\mu^+ - \mu^-} \frac{[(\mu^+)^n - (\mu^-)^n]x_1 + [(\mu^-)^{n-1} - (\mu^+)^{n-1}]x_0}{\eta^2 \neq 1}. \quad (37)$$

For the case when  $\eta^2 < 1$  we write  $\eta = \cos(\theta)$  and then we find

$$x_n = \frac{c}{\sin(\theta)} \frac{\sin(n\theta)x_1 - \sin((n-1)\theta)x_0}{\sin(\theta)} \quad (38)$$

whereas for  $\eta^2 > 1$  we write  $\eta = \cosh(\chi)$  (assuming  $\eta > 1$ ), and then

$$x_n = \frac{c}{\sinh(\chi)} \frac{\sinh(n\chi)x_1 - \sinh((n-1)\chi)x_0}{\sinh(\chi)} \quad (39)$$

and similarly for  $\eta < -1$ . The crucial result is that bounded, elliptic behaviour occurs when  $\eta^2 < 1$  whereas unbounded (hyperbolic) behaviour occurs when  $\eta^2 > 1$ . This result gives a natural cut-off to particle momentum in field theory, as shown in paper II.

The readily solved case when  $\eta^2 = 1$  corresponds to the free particle and will be referred to as the *parabolic* case. When  $\eta^2 > 1$  the system will be said to be *hyperbolic* and *elliptic* when  $\eta^2 < 1$ .

For the case  $\eta^2 < 1$  it is useful to define  $\mu = \eta + i\sqrt{1 - \eta^2}$  and

$$a_n \equiv \mu^n [x_{n+1} - \mu x_n] \quad a_n^* \equiv \mu^{-n} [x_{n+1} - \mu^{-1} x_n] \quad (40)$$

the advantage being that these are constants of motion, namely

$$a_n = a_{n-1} \quad a_n^* = a_{n-1}^*. \quad (41)$$

These are useful when constructing particle states in quantum field theory because they correspond to annihilation and creation operators in the Schrödinger picture.

### 5.3. The Newtonian oscillator

Using the methods outlined in section 3, the continuous time Lagrangian for the Newtonian harmonic oscillator

$$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2 \quad (42)$$

gives the system function

$$F^n = \frac{m(x_{n+1} - x_n)^2}{2T} - \frac{Tm\omega^2}{6} (x_{n+1}^2 + x_{n+1}x_n + x_n^2) \quad (43)$$

which is equivalent to (29). The equation of motion is given by

$$\frac{(x_{n+1} - 2x_n + x_{n-1}))}{T^2} = -\omega^2 \frac{(x_{n+1} + 4x_n + x_{n-1}))}{6} \quad (44)$$

which is equivalent to (30) with the identification  $T^2\omega^2 = 6(1 - \eta)/(2 + \eta)$ , which means

$$\eta = \frac{6 - 2T^2\omega^2}{6 + T^2\omega^2}. \quad (45)$$

Using the results of the previous section, we deduce that elliptic behaviour occurs only when the time  $T$  satisfies the condition

$$0 < T\omega < 2\sqrt{3}. \quad (46)$$

An equivalent result is found in particle field theory, giving a natural cut-off for particle momentum.

### 5.4. Harmonic recurrence

We may understand the relationship between Hamilton's principal function for the interval  $[0, T]$  and the system function by explicitly evaluating the former for the continuous time harmonic oscillator Lagrangian (42). We find

$$S^n(T) = \frac{m\omega}{2 \sin(\omega T)} [(x_{n+1}^2 + x_n^2) \cos(\omega T) - 2x_n x_{n+1}] \quad (47)$$

and comparing this with (43) we find

$$S^n(T) = F^n + O(T^3). \quad (48)$$

We expect a similar relation to exist in the general case, but different potentials will modify the precise details.

There is an apparent problem with (47), whenever the time interval  $T$  satisfies the condition  $\omega T = r\pi$ ,  $r = 1, 2, \dots$  because the denominator  $\sin(\omega T)$  vanishes at such times.

This problem is an artefact of our representation of  $S^n$ , because the definition of the principal function as a line integral over a finite contour of a bounded integrand means that  $S^n$  cannot diverge. The resolution of this apparent paradox is that at the *recurrence times*  $T = r\pi/\omega$  the endpoints  $x_n$  and  $x_{n+1}$  are no longer independent but are related by

$$x_{n+1} = (-1)^r x_n. \quad (49)$$

The physical interpretation of recurrence is simple. The harmonic oscillator has a fundamental period  $P = 2\pi/\omega$ , independent of the initial conditions.

An important construction for the harmonic oscillator are the variables  $A_n, A_n^*$  defined by

$$\begin{aligned} A_n &\equiv \frac{ie^{in\theta}}{\sin(\theta)} [x_{n+1} - e^{i\theta} x_n] \\ A_n^* &\equiv \frac{-ie^{-in\theta}}{\sin(\theta)} [x_{n+1} - e^{-i\theta} x_n] \quad \theta \equiv \omega T. \end{aligned} \quad (50)$$

These are constants of motion, i.e.  $A_n = A_{n+1}$  and are independent of  $T$ . This means that recurrence must occur so as to cancel the zero of the denominator in (47) at the recurrence times. To see what happens explicitly, we may invert equations (50) to find

$$x_n = \frac{1}{2} [e^{in\theta} A_n^* + e^{-in\theta} A_n] \quad x_{n+1} = \frac{1}{2} [e^{i(n+1)\theta} A_n^* + e^{-i(n+1)\theta} A_n] \quad (51)$$

so that at the recurrence times  $T = r\pi/\omega$  we have

$$x_n = \frac{(-1)^{nr}}{2} [A_n^* + A_n] \quad (52)$$

from which we deduce (49).

In terms of  $A_n$  and  $A_n^*$  the principal function can be written as

$$S^n(T) = -\frac{m\omega \sin(\theta)}{4} [e^{i(2n+1)\theta} A_n^{*2} + e^{-i(2n+1)\theta} A_n^2] \quad (53)$$

a form which shows clearly that the principal function is not singular. Moreover, we see that at the recurrence times

$$S^n\left(\frac{r\pi}{\omega}\right) = 0 \quad r = 1, 2, \dots \quad (54)$$

It is a significant feature of the discrete time harmonic oscillator that it does not involve recurrence phenomena in this particular way, as no apparent singularities occur in the system function (43). This emphasizes that discrete time mechanics is not equivalent to continuous time mechanics.

## 6. Electrodynamics: test particles

We now consider the case of electrically charged particles interacting with electromagnetic fields. A more complete discussion of discrete time Maxwell's equations is given in paper II of this series. Here we discuss only the case of test particles which are affected by external electric and magnetic fields but do not affect them. We shall find the Cadzow equation of motion for such particles and show that in our prescription electric charge is conserved.

Consider a non-relativistic charged test particle of mass  $m$  in external electromagnetic potentials. The continuous time Lagrangian for such a system is given by

$$L_{EM} = \frac{1}{2} m \dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + q \dot{\mathbf{x}} \cdot \mathbf{A}(\mathbf{x}, t) - q\phi(\mathbf{x}, t) \quad (55)$$

where  $q$  is the charge of the particle. This Lagrangian is not gauge invariant but the equations of motion are gauge invariant, because under the gauge transformation

$$\begin{aligned}\phi &\rightarrow \phi' \equiv \phi + \partial_t \chi \\ \mathbf{A} &\rightarrow \mathbf{A}' \equiv \mathbf{A} - \nabla \chi\end{aligned}\quad (56)$$

the action integral transforms according to the rule

$$A_{if} \rightarrow A'_{if} \equiv A_{if} - [q\chi]_{t_i}^{t_f} \quad (57)$$

that is, the change in the action integral occurs only at the endpoints. If this property is preserved in any discretized version of electrodynamics then the equations of motion should be gauge invariant. Our prescription for calculating the system function from the Lagrangian does indeed preserve this property and therefore our discrete time equations of motion are gauge invariant.

The first step is to construct discrete time electromagnetic potentials. These are discussed in full detail in paper II, but the basic properties are the following. The magnetic vector potential,  $\mathbf{A}$ , differs from the scalar potential,  $\phi$ , in that the former is defined at temporal lattice sites whereas the latter is defined on the links between these sites. If  $\mathbf{A}_n(\mathbf{x})$  is the value of the vector potential at time  $n$  at position  $\mathbf{x}$ , and  $\phi_n(\mathbf{x})$  is the scalar potential on the link at position  $\mathbf{x}$  from time  $n$  to time  $n+1$ , then under a discrete time gauge transformation we have

$$\begin{aligned}\phi'_n(\mathbf{x}) &= \phi_n(\mathbf{x}) + \frac{\chi_{n+1}(\mathbf{x}) - \chi_n(\mathbf{x})}{T} \\ \mathbf{A}'_n(\mathbf{x}) &= \mathbf{A}_n(\mathbf{x}) - \nabla \chi_n(\mathbf{x})\end{aligned}\quad (58)$$

where  $\chi_n(\mathbf{x})$  is the value of the gauge transformation function at time  $n$  and position  $\mathbf{x}$ . The electric and magnetic fields are defined by

$$\begin{aligned}\mathbf{E}_n(\mathbf{x}) &= -\nabla \phi_n(\mathbf{x}) - \frac{\mathbf{A}_{n+1}(\mathbf{x}) - \mathbf{A}_n(\mathbf{x})}{T} \\ \mathbf{B}_n(\mathbf{x}) &= \nabla \times \mathbf{A}_n(\mathbf{x}).\end{aligned}\quad (59)$$

These are discrete time gauge invariant. By inspection the electric field is associated with temporal links whereas the magnetic field is associated with temporal sites.

In order to apply our discretization prescription to (55) we specify the virtual paths between times  $t_n$  and  $t_{n+1}$  to be given by

$$\begin{aligned}\tilde{\mathbf{x}}_n &\equiv \lambda \mathbf{x}_{n+1} + \bar{\lambda} \mathbf{x}_n \\ \tilde{\mathbf{A}}_n(\tilde{\mathbf{x}}_n) &\equiv \lambda \mathbf{A}_{n+1}(\tilde{\mathbf{x}}_n) + \bar{\lambda} \mathbf{A}_n(\tilde{\mathbf{x}}_n) \\ \tilde{\phi}_n(\tilde{\mathbf{x}}_n) &\equiv \phi_n(\tilde{\mathbf{x}}_n)\end{aligned}\quad (60)$$

and then the system function is given by

$$F^n = \frac{m(\mathbf{x}_{n+1} - \mathbf{x}_n)^2}{2T} + q(\mathbf{x}_{n+1} - \mathbf{x}_n) \cdot \int_0^1 d\lambda \tilde{\mathbf{A}}_n(\tilde{\mathbf{x}}_n) - Tq \int_0^1 d\lambda \tilde{\phi}_n(\tilde{\mathbf{x}}_n). \quad (61)$$

Under a gauge transformation we find

$$F^{n'} = F^n + q\chi_n(\mathbf{x}_n) - q\chi_{n+1}(\mathbf{x}_{n+1}) \quad (62)$$

and so the action sum  $A^N \equiv \sum_{n=0}^{N-1} F^n$  changes according to the rule

$$A^{N'} = A^N + q\chi_0 - q\chi_N \quad (63)$$

in agreement with (57). Therefore, we expect Cadzow's equations of motion, obtained from (61), to be gauge invariant.

In general, the integrals over the external electromagnetic potentials in (61) give complicated equations of motion and we will normally have only an implicit equation for  $\mathbf{x}_{n+1}$ , which however will be gauge invariant. We find

$$\begin{aligned} \frac{m(\mathbf{x}_{n+1} - 2\mathbf{x}_n + \mathbf{x}_{n-1})}{T^2} &= q \int_0^1 d\lambda \{ \bar{\lambda} \mathbf{E}_n(\tilde{\mathbf{x}}_n) + \lambda \mathbf{E}_{n-1}(\tilde{\mathbf{x}}_{n-1}) \} \\ &+ q \frac{(\mathbf{x}_{n+1} - \mathbf{x}_n)}{T} \int_0^1 d\lambda \{ \lambda \bar{\lambda} \mathbf{B}_{n+1}(\tilde{\mathbf{x}}_n) + \bar{\lambda}^2 \mathbf{B}_n(\tilde{\mathbf{x}}_n) \} \\ &+ q \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})}{T} \int_0^1 d\lambda \{ \lambda^2 \mathbf{B}_n(\tilde{\mathbf{x}}_{n-1}) + \bar{\lambda} \lambda \mathbf{B}_{n-1}(\tilde{\mathbf{x}}_{n-1}) \}. \end{aligned} \quad (64)$$

In the limit  $T \rightarrow 0$  we recover the usual Lorentz force law

$$m\ddot{\mathbf{x}} = q\mathbf{E} + q\dot{\mathbf{x}} \times \mathbf{B} \quad (65)$$

for those trajectories where the limit exists.

The charge density,  $\rho_n(\mathbf{x})$ , and current density,  $\mathbf{j}_n(\mathbf{x})$ , are defined by the following functional derivatives with respect to the electromagnetic potentials of the action sum,  $A^N$ :

$$\rho_n(\mathbf{x}) \equiv \frac{-1}{T} \frac{\delta}{\delta \phi_n(\mathbf{x})} A^N \quad \mathbf{j}_n(\mathbf{x}) \equiv \frac{1}{T} \frac{\delta}{\delta \mathbf{A}_n(\mathbf{x})} A^N. \quad (66)$$

We find

$$\begin{aligned} \rho_n(\mathbf{x}) &= q \int_0^1 d\lambda \delta^3(\tilde{\mathbf{x}}_n - \mathbf{x}) \\ \mathbf{j}_n(\mathbf{x}) &= q \frac{(\mathbf{x}_{n+1} - \mathbf{x}_n)}{T} \int_0^1 d\lambda \bar{\lambda} \delta^3(\tilde{\mathbf{x}}_n - \mathbf{x}) + q \frac{(\mathbf{x}_n - \mathbf{x}_{n-1})}{T} \int_0^1 d\lambda \lambda \delta^3(\tilde{\mathbf{x}}_{n-1} - \mathbf{x}) \end{aligned} \quad (67)$$

which satisfy the discrete time analogue of the equation of continuity

$$\frac{\rho_n(\mathbf{x}) - \rho_{n-1}(\mathbf{x})}{T} + \nabla \cdot \mathbf{j}_n(\mathbf{x}) = 0.$$

## 7. The Grassmannian oscillator

We may apply our methods to the Grassmannian oscillator system, which serves as a prototype model for the Dirac equation studied in paper II. Our model consists of one complex anticommuting degree of freedom,  $\psi$ , with equation of motion

$$i\dot{\psi} = \omega\psi \quad i\dot{\psi}^* = -\omega\psi^*. \quad (68)$$

The Lagrangian giving these equations is

$$L = \frac{1}{2} i\dot{\psi}^* \dot{\psi} - \frac{1}{2} i\dot{\psi} \dot{\psi}^* - \omega\psi^* \psi. \quad (69)$$

Equations (68) imply the harmonic oscillator equations of motion

$$\frac{d^2}{dt^2} \psi = -\omega^2 \psi \quad \frac{d^2}{dt^2} \psi^* = -\omega^2 \psi^*. \quad (70)$$

Now consider discretization using the linear virtual paths

$$\tilde{\psi} = \lambda\psi_{n+1} + \bar{\lambda}\psi_n \quad \tilde{\psi}^* = \lambda\psi_{n+1}^* + \bar{\lambda}\psi_n^*. \quad (71)$$

Using (69) we find that the system function is

$$F^n = \frac{1}{2} i[\psi_n^* \psi_{n+1} - \psi_{n+1}^* \psi_n] - \omega T \frac{\{2\psi_{n+1}^* \psi_{n+1} + \psi_n^* \psi_{n+1} + \psi_{n+1}^* \psi_n + 2\psi_n^* \psi_n\}}{6} \quad (72)$$

which leads to the equation of motion

$$i \frac{(\psi_{n+1} - \psi_{n-1})}{2T} = \omega \frac{(\psi_{n+1} + 4\psi_n + \psi_{n-1})}{6} \quad (73)$$

and similarly for the complex conjugate. It does not seem possible to use (73) to obtain the discretization (44) of the harmonic oscillator unless we change the virtual paths or renormalize the frequency  $\omega$ . However, we can readily show that (73) implies harmonic oscillator behaviour by the following method.

First, rewrite (73) as

$$(-3i + \kappa)\psi_{n+1} + (3i + \kappa)\psi_{n-1} = -4\kappa\psi_n \quad (74)$$

where  $\kappa \equiv \omega T$ . If we define

$$v \equiv \frac{3i + \kappa}{\sqrt{9 + \kappa^2}} \quad v^{-1} \equiv \frac{-3i + \kappa}{\sqrt{9 + \kappa^2}} \quad (75)$$

and shift the degrees of freedom according to the rule

$$\psi_n \equiv v^n \phi_n \quad (76)$$

then the variables  $\phi_n$  satisfy the discrete time oscillator equation

$$\phi_{n+1} + \phi_{n-1} = 2\eta\phi_n \quad (77)$$

where  $\eta = \frac{-2\kappa}{\sqrt{9 + \kappa^2}}$ . We find

$$\mu \equiv \eta + i\sqrt{1 - \eta^2} = \frac{-2\kappa + i\sqrt{9 - 3\kappa^2}}{\sqrt{9 + \kappa^2}} \quad (78)$$

from which we deduce the upper limit  $\omega T < \sqrt{3}$  for elliptic behaviour in the system. This is exactly one half of the upper limit found for the bosonic discrete time oscillator.

## 8. First quantization

We now discuss the possibility of quantizing our classical discrete time mechanics. If we denote the process of quantization by the symbol  $\mathcal{Q}$  and the process of discretization by the symbol  $\mathcal{D}$  then the question arises, do these processes commute, i.e. does  $\mathcal{Q}\mathcal{D} \stackrel{?}{=} \mathcal{D}\mathcal{Q}$ . In other words, does it matter if we discretize the quantum theory of some system with classical Lagrangian rather than quantize the discretized version of the same classical Lagrangian?

There is *a priori* no reason to expect these processes to commute. For one thing, we have not yet decided what  $\mathcal{Q}$  might mean. Also, there are some aspects of  $\mathcal{D}$  such as the lack of a Hamiltonian which makes a dynamical quantum theory of discrete time point particle mechanics problematical. Fortunately, there are some concepts from the conventional  $\mathcal{Q}$  programme which are useful and appear to survive  $\mathcal{D}$ . We shall comment on some of these aspects now and then consider the harmonic oscillator quantization process  $\mathcal{Q}\mathcal{D}$  in some detail in the following sections, saving a discussion of the  $\mathcal{D}\mathcal{Q}$  process until paper II.

In the following we discuss a system consisting of a point particle in one dimension. Generalization to more degrees of freedom is straightforward and we shall use the Dirac bra-ket notation for convenience.

### 8.1. Basics

In our approach to quantization, we shall follow all the standard principles of orthodox quantum mechanics in the main. This means we face the same issues of rigour and interpretation as orthodox quantum theory. We shall not comment on those in general. We discuss below those aspects where discretization of time requires some additional emphasis or comment.

*Proposition 1.* Physical states of a quantum system correspond one-to-one to rays in a separable Hilbert space,  $\mathcal{H}$ . A physical state vector  $|\phi\rangle$  will be in general normalized to unity, namely

$$\langle\phi|\phi\rangle = 1. \quad (79)$$

*Proposition 2.* For each integer time  $n$  (or more accurately, at each coordinate time  $nT$ ),  $\mathcal{H}$  is spanned by an improper basis  $\mathcal{B}^n \equiv \{|x, n\rangle : x \in \mathfrak{R}\}$ , the elements of which satisfy the relation

$$\langle x, n|y, n\rangle = \delta(x - y). \quad (80)$$

The resolution of the identity operator in  $\mathcal{H}$  is

$$\hat{I}_{\mathcal{H}} = \int dx |x, n\rangle\langle x, n| \quad (81)$$

which holds for each  $n$ .

Given a physical state  $|\psi\rangle$  in  $\mathcal{H}$  we may write for each  $n$

$$|\psi\rangle = \int dx \psi_n(x)|x, n\rangle \quad (82)$$

where  $\psi_n(x)$  is the wavefunction at time  $n$ , with the property that

$$\int dx |\psi_n(x)|^2 = 1 \quad (83)$$

assuming normalization to unity.

*Remark 1.* The Heisenberg picture is being used in the above. The time dependence of the basis sets  $\mathcal{B}^n$  allows us to use the Schrödinger picture, discussed below.

*Remark 2.* All the usual principles of quantum mechanics concerning the interpretation of the states in the Hilbert space apply here. For example, (a) the superposition principle and its interpretation according to standard quantum mechanics holds and (b) given two physical states  $|\phi\rangle$ ,  $|\psi\rangle$  then the inner product  $\langle\phi|\psi\rangle$  gives the conditional transition amplitude for the system to be found in state  $|\phi\rangle$ , given it is in state  $|\psi\rangle$ .

*Definition 1.* An operator  $\hat{A}$ , diagonal with respect to  $\mathcal{B}^n$ , is one which can be written in the form

$$\hat{A} = \int dx |x, n\rangle A(x, \partial_x)\langle x, n| \quad (84)$$

where the component operator  $A(x, \partial_x)$  is some differential operator of finite order.

The action of such an operator on a typical state  $|\psi\rangle$  is given by

$$|A\psi\rangle \equiv \hat{A}|\psi\rangle = \int dx |x, n\rangle A(x, \partial_x)\psi_n(x) \quad (85)$$

with matrix elements given by

$$\langle\phi|A\psi\rangle = \int dx \phi^*(x)A(x, \partial_x)\psi_n(x). \quad (86)$$



*Remark 3.* The wavefunctions of the theory are elements of  $\mathcal{L}^2(\mathfrak{R})$ , the space of square integrable functions on  $\mathfrak{R}$ , and the operators (including the observables of the theory) which act on them are usually built up of functions of  $x$  and  $\partial_x$ . If at a given time,  $n$ , the component operator of some observable diagonal with respect to  $\mathcal{B}^n$  happens to be represented by say a multiple of  $\partial_x$  this carries no implication that the observable is related to a velocity (which would normally be implied in conventional wave mechanics, where the momentum operator is represented by  $-i\hbar\partial_x$ ). There is no concept of velocity in the normal sense in discrete time mechanics.

Keeping in mind the caveats discussed in [12] concerning Hermitian and adjoint operators, we define the Hermitian conjugate or adjoint operator  $\hat{A}^+$  to have the property that

$$\langle\phi|A\psi\rangle = \langle\psi|\hat{A}^+\phi\rangle^* \quad (87)$$

for a dense set of physical states. If  $\hat{A}$  is diagonal with respect to  $\mathcal{B}^n$  then assuming we may represent  $\hat{A}^+$  in the form

$$\hat{A}^+ = \int dx |x, n\rangle \tilde{A}(x, \partial_x) \langle x, n| \quad (88)$$

for some operator component  $\tilde{A}(x, \partial_x)$  we find

$$\int dx \phi_n^*(x) A(x, \partial_x) \psi_n(x) = \int dx [\tilde{A}^*(x, \partial_x) \phi_n^*(x)] \psi_n(x). \quad (89)$$

Assuming that we are permitted to integrate by parts, which will be the case for normalizable wavefunctions falling off at spatial infinity, we can readily understand the relationship between  $A(x, \partial_x)$  and  $\tilde{A}(x, \partial_x)$ . Given the former we can always work out the latter by integration by parts and vice versa.

If  $A(x, \partial_x) = \tilde{A}(x, \partial_x)$  then  $\hat{A} = \hat{A}^+$  and the operator is self-adjoint. Physical observables of the theory which are diagonal with respect to  $\mathcal{B}^n$  will be assumed to have this property.

## 8.2. Dynamics

The dynamical content of the theory is expressed in terms of unitary *timestep operators*,  $\hat{U}_n$ , one for each  $n$ .

*Proposition 3.* For each  $n$  there is a unitary operator,  $\hat{U}_n$ , such that

$$|x, n+1\rangle = \hat{U}_n^\dagger |x, n\rangle. \quad (90)$$

From this we deduce the relations

$$\begin{aligned} \langle x, n+1| &= \langle x, n| \hat{U}_n \\ |x, n\rangle &= \hat{U}_n |x, n+1\rangle \\ \langle x, n| &= \langle x, n+1| \hat{U}_n^\dagger. \end{aligned} \quad (91)$$

*Remark 4.* The operator  $\hat{U}_n$  provides an isometry between  $\mathcal{B}^n$  and  $\mathcal{B}^{n+1}$ , that is

$$\langle x, n+1|y, n+1\rangle = \langle x, n|y, n\rangle = \delta(x-y). \quad (92)$$

Using the resolution of identity (81) we may represent the timestep operators in the non-diagonal form

$$\hat{U}_n = \int dx |x, n\rangle \langle x, n+1| \quad \hat{U}_n^\dagger = \int dx |x, n+1\rangle \langle x, n|. \quad (93)$$

We are now in a position to define the fundamental functions of the quantum theory, the *system amplitudes*  $U_n(x, y)$ , defined by

$$\begin{aligned} U_n(x, y) &\equiv \langle x, n+1 | y, n \rangle = \langle x, n | \hat{U}_n | y, n \rangle \\ U_n^*(x, y) &\equiv \langle y, n | x, n+1 \rangle = \langle y, n | \hat{U}_n^\dagger | x, n \rangle \end{aligned} \quad (94)$$

from which we arrive at the non-diagonal expressions

$$\begin{aligned} \hat{U}_n &= \int dx dy |x, n\rangle U_n(x, y) \langle y, n| \\ \hat{U}_n^\dagger &= \int dx dy |x, n\rangle U_n^*(y, x) \langle y, n|. \end{aligned} \quad (95)$$

*Remark 5.* The system amplitudes will not be differential operators of finite order in general but well behaved complex-valued functions of two real variables. Neither will they be singular distributions. They are similar in function to integrated Feynman transition kernels encountered in the path integral formulation of standard quantum mechanics.

The condition that the timestep operators are unitary, namely

$$\hat{U}_n \hat{U}_n^\dagger = \hat{I}_{\mathcal{H}} \quad (96)$$

leads to the closure condition

$$\int dy U_n(x, y) U_n^*(z, y) = \delta(x - z) \quad (97)$$

on the system amplitudes.

*Definition 2.* A system for which the system amplitudes are independent of time, such that we may write

$$U_n(x, y) = U(x, y) \quad (98)$$

for some  $U(x, y)$  and for all  $n$ , will be said to be *autonomous*.

*Definition 3.* An autonomous system for which the system amplitude  $U(x, y)$  carries the symmetry

$$U(x, y) = U(y, x) \quad (99)$$

will be said to be *time-reversal invariant*.

*Remark 6.* Most of the system amplitudes of interest to us will be autonomous and time-reversal invariant. This will be so whenever we construct system amplitudes from system functions which have been obtained from conventional time-translation invariant and time-reversal invariant Lagrangians using the virtual path approach discussed above.

### 8.3. The Schrödinger picture

The Heisenberg picture description of the physical states used so far means that we may write

$$|\psi\rangle = \int dx \psi_{n+1}(x) |x, n+1\rangle = \int dx \psi_n(x) |x, n\rangle \quad (100)$$

from which we deduce

$$\psi_{n+1}(x) = \int dy U_n(x, y) \psi_n(y). \quad (101)$$

From this we see that the system amplitudes play a role analogous to finite time scattering kernels in conventional quantum mechanics. Equation (101) is about the closest we come in this theory to something analogous to a time-dependent Schrödinger wave equation.

We may set up a formal description in the Schrödinger picture as follows. Given a Heisenberg picture state  $|\psi\rangle$  and a knowledge of the component functions  $\psi_n(x)$ , define the sequence of states

$$|\psi_{n,m}\rangle \equiv \int dx \psi_n(x) |x, m\rangle \quad (102)$$

for some chosen time  $m$ . Then if  $|\psi_{m,m}\rangle \equiv |\psi\rangle$  we find

$$\hat{U}_m |\psi_{m,m}\rangle = |\psi_{m+1,m}\rangle. \quad (103)$$

It is straightforward to extend this to jumps over more than one time interval. This establishes the Schrödinger picture in this theory.

#### 8.4. Position eigenstates

Given an improper basis  $\mathcal{B}^n \equiv \{|x, n\rangle : x \in \mathfrak{R}\}$  we may construct a self-adjoint position operator

$$\hat{x}_n \equiv \int dx |x, n\rangle x \langle x, n| \quad (104)$$

which has the property

$$\hat{x}_n |x, n\rangle = x |x, n\rangle. \quad (105)$$

*Remark 7.* For convenience we shall follow the traditional abuse of notation and use the symbol  $x$  for both the position operator and a particular eigenvalue of that operator. It will be clear normally from the context what is meant whenever a clash of notation occurs.

The position operators have the merit of being diagonal with respect to the appropriate basis, that is,  $\hat{x}_n$  is diagonal with respect to  $\mathcal{B}^n$ . The position operators are not necessarily diagonal with respect to bases at other values of  $n$ . From the condition

$$\hat{x}_{n+1} = \hat{U}_n^\dagger \hat{x}_n \hat{U}_n \quad (106)$$

we find

$$\hat{x}_{n+1} = \int dx dy dz |x, n\rangle U_n^*(y, x) y U_n(y, z) \langle z, n| \quad (107)$$

which is self-adjoint but not necessarily diagonal with respect to  $\mathcal{B}^n$ .

*Remark 8.* It is possible for  $\hat{x}_{n+1}$  to reduce to diagonal form with respect to the  $\mathcal{B}^n$  basis but this depends on the details of the system amplitudes.

From the above we arrive at the fundamental expression for the commutators:

$$[\hat{x}_{n+1}, \hat{x}_n] = \int dx dy dz |x, n\rangle U_n^*(y, x) y (z - x) U_n(y, z) \langle z, n|. \quad (108)$$

## 8.5. Normal coordinate systems

In this section we discuss the quantization of a large family of systems for which the following property holds.

*Definition 4.* Coordinates for a system for which the right-hand side of the commutator (108) is a multiple of the identity operator for each value of  $n$  will be called *normal*.

*Remark 9.* We shall see below that the coordinates for the important system equivalent to the harmonic oscillator are normal.

A class of system amplitudes for which the coordinates are normal may be constructed from autonomous, time-reversal invariant system functions of the form

$$F(x_n, x_{n+1}) = -\beta x_n x_{n+1} + \frac{1}{2} W(x_n) + \frac{1}{2} W(x_{n+1}) \quad (109)$$

where  $\beta$  is a non-zero constant. The Cadzow's equation for this system is

$$x_{n+1} = \beta^{-1} W'(x_n) - x_{n-1} \quad (110)$$

which has the merit of giving  $x_{n+1}$  explicitly in terms of  $x_n$  and  $x_{n-1}$ .

Now define the system amplitude to be given by

$$U_n(x, y) = k e^{iF(x,y)/\hbar} \quad (111)$$

where  $k$  is some constant. Then from the unitarity condition (97) we find

$$|k|^2 = \frac{\beta}{2\pi\hbar}. \quad (112)$$

From (108) we find

$$[\hat{x}_{n+1}, \hat{x}_n] = \frac{-i\hbar}{\beta} \quad (113)$$

so that the above coordinates for this system are normal. Moreover, with the momentum,  $p_n$ , conjugate to  $x_n$  defined by (10), we recover the conventional commutator

$$[\hat{p}_n, \hat{x}_n] = -i\hbar. \quad (114)$$

This result is not expected to hold for systems which are not normal.

The operator equations of motion are found to be

$$\hat{x}_{n+1} = \beta^{-1} \hat{W}'_n - \hat{x}_{n-1} \quad (115)$$

where  $\hat{W}'$  is the diagonal operator

$$\hat{W}'_n \equiv \int dx |x, n\rangle \left\{ \frac{dW(x)}{dx} \right\} \langle x, n|. \quad (116)$$

From this we obtain the discrete time version of Ehrenfest's theorem; i.e.

$$\langle \hat{x}_{n+1} \rangle = \beta^{-1} \langle \hat{W}'_n \rangle - \langle \hat{x}_{n-1} \rangle \quad (117)$$

for expectation values over a physical state.

## 8.6. Compatible operators

In our theory the quantum dynamics is completely determined by the system amplitude. Suppose now that the system is autonomous and time-reversal invariant. This means that for each time  $n$  we may write

$$U_n(x, y) = U(x, y) \quad (118)$$

where  $U(x, y)$  is independent of  $n$ . For such a system there may be constants of motion comparable with the Maeda–Noether and Logan invariants discussed in the classical theory.

Consider an operator,  $\hat{C}$ , diagonal with respect to  $\mathcal{B}^n$ , namely

$$\hat{C} \equiv \int dx |x, n\rangle C(x, \partial_x) \langle x, n| \quad (119)$$

where  $C(x, \partial_x)$  is some differential operator of finite order. Matrix elements of the commutator of  $\hat{C}$  with  $\hat{U}$  are given by

$$\langle \phi | [\hat{C}, \hat{U}] | \psi \rangle = \int dx dy \phi_n^*(x) \{ C(x, \partial_x) U(x, y) - \tilde{C}^*(y, \partial_y) U(x, y) \} \psi_n(y) \quad (120)$$

where  $|\psi\rangle$  and  $|\phi\rangle$  are arbitrary physical states. From this we arrive at the following result

*Theorem.* A diagonal operator commutes with the timestep operator of an autonomous system if

$$C(x, \partial_x) U(x, y) = \tilde{C}^*(y, \partial_y) U(x, y). \quad (121)$$

*Definition 5.* A diagonal operator which commutes with the timestep operator of an autonomous system will be said to be *compatible* (with the timestep operator).

*Remark 10.* It is not necessary for a diagonal operator,  $\hat{C}$ , to be self-adjoint for it to be compatible with the timestep operator.

*Remark 11.* From the above we deduce that compatible operators are invariants of motion. To be explicit, consider a state  $|\psi\rangle$  which is an eigenstate of the diagonal operator,  $\hat{C}$ , with eigenvalue  $c$ , i.e.

$$\hat{C}|\psi\rangle = c|\psi\rangle. \quad (122)$$

Then we can show

$$C(x, \partial_x) \psi_n(x) = c \psi_n(x) \quad (123)$$

and

$$C(x, \partial_x) \psi_{n+1}(x) = c \psi_{n+1}(x). \quad (124)$$

*Remark 12.* Given the system amplitude  $U(x, y)$  it may be very hard or perhaps even impossible to find any compatible operators in closed form. It may be necessary to approximate such an operator via a perturbative expansion, for example. This is the quantum theory analogue of the problem of finding invariants of motion for a classical discrete time theory given some system function.

*Remark 13.* Discrete time and continuous time quantum mechanics pose dual problems in the following sense. In continuous time quantum mechanics we are normally given a Hamiltonian and the problem is to construct the time evolution operator. For a time-independent Hamiltonian a complete solution would require us to find all the eigenvalues

$E_\alpha$  and eigenstates  $|E_\alpha\rangle$  of  $\hat{H}$  and then use them in the formal solution  $\hat{U}_t = \exp\{-i\hat{H}t/\hbar\}$  to write

$$\hat{U}_t = \sum_\alpha |E_\alpha\rangle e^{-iE_\alpha t/\hbar} \langle E_\alpha|. \quad (125)$$

This is, in general, a formidable problem. In discrete time quantum mechanics the situation is the other way around. Given a system amplitude, the problem is to find the compatible operators, if any. An important system where answers can be found to all of these questions in both approaches is the discrete time harmonic oscillator discussed in section 10.

## 9. Stroboscopic construction

In principle it should always be possible to construct examples of discrete time quantum systems by integrating the equation

$$i\hbar \partial_t \hat{U}(t) = \hat{H} \hat{U}(t) \quad (126)$$

for the evolution operator  $\hat{U}(t)$  in continuous time quantum mechanics, given the Hamiltonian  $\hat{H}$ . The boundary condition

$$\lim_{t \rightarrow 0} \hat{U}(t) = \hat{I}_\mathcal{H} \quad (127)$$

ensures a unique solution. From this point of view the discussion outlined above represents a stroboscopic approach, where the state vectors evolve continuously but are looked at periodically in a non-destructive (mathematical) sense. This examination of the state vector is *not* the same as an observation collapsing the wavefunction.

For autonomous systems a formal solution to (126) is

$$\hat{U}(t) \equiv \exp(-i\hat{H}t/\hbar). \quad (128)$$

In this approach the transition amplitude  $U(x, y; t) \equiv \langle x, t | y, 0 \rangle$  corresponds to our system amplitude when  $t = T$  and may be evaluated in a number of ways. For example, the Feynman path integral method gives the formula

$$\langle x, t | y, 0 \rangle \sim \int [dz] \exp \left\{ \frac{i}{\hbar} \int_0^t dt' L(\dot{z}, z, t') \right\} \quad t > 0 \quad (129)$$

where  $L$  is the Lagrangian, such amplitudes being functions of  $t$  and the endpoints  $x$  and  $y$ . The standard approach to the evaluation of such integrals is, rather interestingly, based on the discretization of time. The time interval  $[0, t]$  is partitioned into a finite number  $N$  of equal steps, the integrand in the exponential is approximated suitably (by what amounts to choosing a virtual path in our approach), the  $N$  integrals are evaluated, and then the limit  $N \rightarrow \infty$  taken.

The relationship between this approach and our discrete time formalism should now be clear, the basic difference being that we do not take the limit  $N \rightarrow \infty$ . In a number of situations our system amplitude will actually take the form

$$U(x, y) \equiv \langle x, T | y, 0 \rangle \sim \exp\{iF(x, y)/\hbar\} \quad (130)$$

and then for  $N$  timesteps the transition amplitude  $\langle x, NT | y, 0 \rangle$  becomes

$$\langle x, NT | y, 0 \rangle \sim \int \dots \int dx_1 dx_2 \dots dx_{N-1} \exp\{iA^N/\hbar\} \quad (131)$$

which emphasizes the relationship further.

An important point which could be confusing is that the system function in (130) does *not* correspond to a Logan constant for those systems such as the harmonic oscillator where

such an invariant can be found. System functions in general are not expected to be invariants of motion.

An alternative method of constructing the transition amplitudes is to find the Green's functions for the system. If the transition amplitude  $U(x, y; t)$  satisfies the homogeneous Schrödinger equation

$$(i\hbar\partial_t - \vec{H}_x)U(x, y, t) = 0 \quad (132)$$

with the boundary condition

$$\lim_{t \rightarrow 0} U(x, y, t) = \delta^3(\mathbf{x}) \quad (133)$$

then the retarded and advanced Green's functions  $G_R(x, y, t)$  and  $G_A(x, y, t)$  are related to the transition amplitude by

$$\begin{aligned} G_R(x, y, t) &= \theta(t)U(x, y, t) \\ G_A(x, y, t) &= -\theta(-t)U(x, y, t) \end{aligned} \quad (134)$$

and these satisfy the inhomogeneous equation

$$(i\hbar\partial_t - \vec{H}_x)G(x, y, t) = i\hbar\delta(t)\delta^3(\mathbf{x}). \quad (135)$$

If we can solve this equation, we can immediately construct the transition amplitude using the relation

$$U(x, y, t) = G_R(x, y, t) - G_A(x, y, t). \quad (136)$$

### 9.1. Example: the free Newtonian particle

Given the Hamiltonian

$$H = \frac{\mathbf{p} \cdot \mathbf{p}}{2m} \quad (137)$$

in continuous time mechanics we can readily find the Green's functions in the quantum theory. We find

$$\begin{aligned} G_R(\mathbf{x}, \mathbf{y}, t) &= \theta(t) \left( \frac{-im}{2\pi\hbar t} \right)^{3/2} \exp \left\{ \frac{i}{\hbar} \frac{m(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2t} \right\} \\ G_A(\mathbf{x}, \mathbf{y}, t) &= -\theta(-t) \left( \frac{-im}{2\pi\hbar t} \right)^{3/2} \exp \left\{ \frac{i}{\hbar} \frac{m(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2t} \right\} \end{aligned} \quad (138)$$

from which we construct the transition amplitude

$$U(\mathbf{x}, \mathbf{y}, t) = \left( \frac{-im}{2\pi\hbar t} \right)^{3/2} \exp \left\{ \frac{i}{\hbar} \frac{m(\mathbf{x} - \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y})}{2t} \right\} \quad t > 0. \quad (139)$$

This satisfies the closure condition (97)

$$\int d^3\mathbf{y} U(\mathbf{x}, \mathbf{y}; T)U^*(\mathbf{z}, \mathbf{y}; T) = \delta^3(\mathbf{x} - \mathbf{z}) \quad (140)$$

for a system amplitude and demonstrates the essential point that it is possible to construct examples of discrete time quantum mechanics from continuous time quantum mechanics. The converse need not be true. Given a system amplitude, it may be impossible to find a compatible operator equivalent to some second-order Hamiltonian operator in continuous time mechanics. It is not difficult to find examples of normal systems where this occurs.

### 10. The discrete time harmonic oscillator

Given the discrete time harmonic oscillator system function

$$F^n \equiv F(x_{n+1}, x_n) = \frac{1}{2}\alpha(x_{n+1}^2 + x_n^2) - \beta x_{n+1}x_n \quad (141)$$

we note that it is an example of a normal system. This leads us to define the system amplitude to be

$$\begin{aligned} U_n(x, y) &= k \exp(iF(x, y)/\hbar) \\ &= k \exp\left(\frac{i}{2\hbar}[\alpha x^2 + \alpha y^2 - 2\beta xy]\right) \end{aligned} \quad (142)$$

where  $k$  is some constant. From the unitarity condition (97) we find (112) and from (108) we find (113), so we see that the above system's coordinates are indeed normal. The self-adjoint diagonal operator with operator component

$$\vec{C}_x \equiv \frac{1}{2}\beta^{-1}[-\hbar^2\partial_x^2 + (\beta^2 - \alpha^2)x^2] \quad (143)$$

is compatible with the system amplitude (142).

The interpretation of this is that  $\vec{C}_x$  is the operator corresponding to the Logan constant for the classical discrete time harmonic oscillator

$$C = \frac{1}{2}\beta(x^2 + y^2) - \alpha xy. \quad (144)$$

To see this explicitly, consider the operators  $\hat{x}_n$  and  $\hat{x}_{n+1}$ . The Logan constant for the harmonic oscillator is quantized according to the standard rule

$$\hat{C} = \frac{1}{2}\beta(\hat{x}_n\hat{x}_n + \hat{x}_{n+1}\hat{x}_{n+1}) - \frac{1}{2}\alpha(\hat{x}_n\hat{x}_{n+1} + \hat{x}_{n+1}\hat{x}_n). \quad (145)$$

A suitable coordinate representation of these operators with respect to the basis  $\mathcal{B}^n$  is

$$\hat{x}_n \rightarrow x \quad \hat{x}_{n+1} \rightarrow \eta x - i\frac{\hbar}{\beta}\partial_x \quad (146)$$

and then operator (145) is represented by (143).

We see from the potential term in the differential operator (143) that a complete set of physical states can be found as eigenstates of the operator provided  $\beta^2 > \alpha^2$ . This corresponds precisely to the elliptic region discussed in the classical theory.

If the constants satisfy the elliptic condition, we may construct annihilation and creation operators for the system. These are diagonal with respect to any of the bases  $\mathcal{B}^n$  and are given by

$$\begin{aligned} \hat{a}_n &\equiv ie^{in\theta}[\hat{x}_{n+1} - e^{i\theta}\hat{x}_n] = e^{in\theta} \int dx |x, n\rangle \left\{ \sqrt{1 - \eta^2}x + \frac{\hbar}{\beta}\partial_x \right\} \langle x, n| \\ \hat{a}_n^+ &\equiv -ie^{-in\theta}[\hat{x}_{n+1} - e^{-i\theta}\hat{x}_n] = e^{-in\theta} \int dx |x, n\rangle \left\{ \sqrt{1 - \eta^2}x - \frac{\hbar}{\beta}\partial_x \right\} \langle x, n|. \end{aligned} \quad (147)$$

These operators satisfy the commutation relation

$$[\hat{a}_n, \hat{a}_n^+] = \frac{2\hbar\sqrt{1 - \eta^2}}{\beta}. \quad (148)$$

Using the evolution relation (106) and the operator equation of motion

$$\hat{x}_{n+1} = 2\eta\hat{x}_n - \hat{x}_{n-1} \quad (149)$$

we find

$$\hat{a}_{n+1} = \hat{a}_n \quad (150)$$



but this does not mean that this operator is conserved. A conserved operator, according to our definition, must be compatible with the timestep operator  $\hat{U}_n$ . We find that the creation and annihilation operators satisfy the relations

$$\begin{aligned}\hat{U}_n \hat{a}_n - e^{i\theta} \hat{a}_n \hat{U}_n &= 0 \\ \hat{U}_n \hat{a}_n^+ - e^{-i\theta} \hat{a}_n^+ \hat{U}_n &= 0\end{aligned}\quad (151)$$

which is reminiscent of various deformed commutators encountered in quantum mechanics. However, operator (145) corresponding to the Logan constant  $C^n = \frac{1}{2}\beta a_n^* a_n$  is compatible with the timestep operator and is therefore an invariant of motion. We find

$$\begin{aligned}\hat{C} &= \frac{1}{4}\beta\{\hat{a}^+ \hat{a} + \hat{a} \hat{a}^+\} = \frac{1}{2}\beta \hat{a}^+ \hat{a} + \frac{1}{2}\sqrt{1-\eta^2}\hbar \\ &= \int dx |x, n\rangle \left\{ \frac{-\hbar^2}{2\beta} \frac{\partial^2}{\partial x^2} + \frac{1}{2}\beta(1-\eta^2)x^2 \right\} \langle x, n| \\ &= \int dx |x, n\rangle \vec{C}_x \langle x, n|.\end{aligned}\quad (152)$$

This Logan invariant is a close analogue of the oscillator Hamiltonian in continuous time mechanics and the eigenstates of the former follow the same pattern as the eigenstates of the latter. For example, there is a ground state  $|\Psi_0\rangle$  satisfying the relation

$$\hat{a}_n |\Psi_0\rangle = 0 \quad (153)$$

with normalizable wavefunction  $\Psi_0(x) = \Psi_0(0) \exp\{-\frac{1}{2}\beta\sqrt{1-\eta^2}x^2/\hbar\}$ . This wavefunction is also an eigenstate of the Logan invariant operator, with

$$\vec{C} \Psi_0(x) = \frac{1}{2}\sqrt{1-\eta^2}\hbar \Psi_0(x). \quad (154)$$

These results hold only for  $|\eta| < 1$ . We note from section 5.3 that  $\beta = m(6+T^2\omega^2)/6T$  and that

$$\lim_{T \rightarrow 0} \frac{\vec{C}}{T} = -\frac{\hbar^2}{2m} \partial_x^2 + \frac{1}{2}m\omega^2 \quad (155)$$

when we identify our system with the Newtonian oscillator.

## 11. The inhomogeneous oscillator

In this section we discuss the inhomogeneous harmonic oscillator, which serves as a prototype for the application of our quantization principles to field theories. We will use the source functional techniques of Schwinger to obtain the ground-state functional and various  $n$ -point functions of interest. Because the Schwinger method deals with time-ordered products we should expect the discretization of the time parameter to involve some changes in the details of the calculations.

First, given a system function  $F^n \equiv F(x_n, x_{n+1})$  we are free to introduce an external source in any convenient way, as ultimately this will be set to zero. Our choice is to define the system function  $F^n[j]$  in the presence of the external source as

$$F^n[j] \equiv F^n + \frac{1}{2}T j_{n+1} x_{n+1} + \frac{1}{2}T j_n x_n \quad (156)$$

a choice which allows the construction of time-ordered product expectation values directly. The action sum from time  $MT$  to time  $NT$  ( $N > M$ ) now becomes

$$A^{NM}[j] = A^{NM} + \frac{1}{2}T j_M x_M + \frac{1}{2}T j_N x_N + T \sum_{n=M+1}^{N-1} j_n x_n \quad M < N \quad (157)$$

from which Cadzow's equation of motion is found to be

$$\frac{\partial}{\partial x_n} \{F^n + F^{n-1}\} + j_n = 0 \quad M < n < N. \quad (158)$$

Quantization is introduced via the Schwinger action principle modified for discrete time. We postulate that for an infinitesimal variation  $\delta \hat{A}^{NM}[j]$  of the action operator then

$$\delta \langle \phi, N | \psi, M \rangle^j = \frac{i}{\hbar} \langle \phi, N | \delta \hat{A}^{NM}[j] | \psi, M \rangle^j \quad M < N \quad (159)$$

for any states  $|\phi, N\rangle$ ,  $|\psi, M\rangle$  at times  $NT$ ,  $MT$  respectively, with evolution in the presence of the source. Independent variation of the  $j_n$  for  $M \leq n \leq N$  then leads to the equations

$$\begin{aligned} \frac{-i\hbar}{T} \frac{\partial}{\partial j_M} \langle \phi, N | \psi, M \rangle^j &= \frac{1}{2} \langle \phi, N | \hat{x}_M | \psi, M \rangle^j \\ \frac{-i\hbar}{T} \frac{\partial}{\partial j_n} \langle \phi, N | \psi, M \rangle^j &= \langle \phi, N | \hat{x}_n | \psi, M \rangle^j \quad M < n < N \quad (160) \\ \frac{-i\hbar}{T} \frac{\partial}{\partial j_N} \langle \phi, N | \psi, M \rangle^j &= \frac{1}{2} \langle \phi, N | \hat{x}_N | \psi, M \rangle^j. \end{aligned}$$

Further application of the principle leads to expectation values of time-ordered product of operators, such as

$$\left(\frac{-i\hbar}{T}\right)^2 \frac{\partial^2}{\partial j_m \partial j_n} \langle \phi, N | \psi, M \rangle^j = \langle \phi, N | \tilde{T} \hat{x}_m \hat{x}_n | \psi, M \rangle^j \quad M < m, n < N \quad (161)$$

where the symbol  $\tilde{T}$  denotes discrete time ordering. For example,

$$\begin{aligned} \tilde{T} \hat{x}_m \hat{x}_n &= (\Theta_{m-n} + \frac{1}{2} \delta_{m-n}) \hat{x}_m \hat{x}_n + (\Theta_{n-m} + \frac{1}{2} \delta_{m-n}) \hat{x}_n \hat{x}_m \\ &= \Theta_{m-n} \hat{x}_m \hat{x}_n + \delta_{m-n} \hat{x}_n \hat{x}_m + \Theta_{n-m} \hat{x}_n \hat{x}_m \end{aligned} \quad (162)$$

where  $\Theta_n$  is the discrete step function, defined by

$$\begin{aligned} \Theta_n &= +1 & n > 0 \\ &= 0 & n \leq 0 \end{aligned} \quad (163)$$

and  $\delta_n$  is the Kronecker delta, defined by

$$\begin{aligned} \delta_n &= +1 & n = 0 \\ &= 0 & n \neq 0. \end{aligned} \quad (164)$$

Given the harmonic oscillator system function

$$F^n = \frac{m(x_{n+1} - x_n)^2}{2T} - \frac{Tm\omega^2}{6}(x_{n+1}^2 + x_{n+1}x_n + x_n^2). \quad (165)$$

the classical discrete time harmonic oscillator in the presence of the external source  $j_n$  satisfies the equation

$$x_{n+1} = \frac{2\eta}{c} x_n - x_{n-1} + \frac{T}{\beta} j_n \quad (166)$$

where  $\eta = \alpha/\beta$  with

$$\alpha = \frac{m(1 - 2T^2\omega^2)}{6T} \quad \beta = \frac{m(6 + T^2\omega^2)}{6T}. \quad (167)$$

As discussed previously, elliptic (oscillatory) solutions occur for  $\eta^2 < 1$  whereas hyperbolic solutions occur for  $\eta^2 > 1$ . We will now discuss these possibilities individually.

### 11.1. The elliptic regime

The importance of the elliptic regime  $\eta^2 < 1$  stems from the fact that in field theory this corresponds to physical particle configurations of the fields, i.e. solutions which can be normalized.

Now define the action of the (classical) discrete time displacement operator,  $U_n$ , by the rule

$$U_n f_n \equiv f_{n+1} \quad (168)$$

for any function of the index  $n$ , where  $n$  is real. Then (166) may be written in the form

$$(U_n - 2\eta + U_n^{-1})x_n = \frac{T}{\beta} j_n. \quad (169)$$

To solve (166) for the elliptic case we first define the following: since  $\eta^2 < 1$  we write  $c \equiv \cos(\theta) = \eta$  and  $s \equiv \sin(\theta) = +\sqrt{1-\eta^2} > 0$ , taking  $0 < \theta < \pi$ . If we define  $s_a \equiv \sin(a\theta)$  where  $a$  is real then a useful identity is

$$s_a s_{b-c} + s_b s_{c-a} + s_c s_{a-b} = 0. \quad (170)$$

From this we deduce

$$s_{a+1} + s_{a-1} = 2cs_a \quad (171)$$

which is equivalent to

$$(U_a - 2\eta + U_a^{-1})s_a = 0. \quad (172)$$

We define the matrices

$$\Lambda^n = \frac{1}{s} \begin{bmatrix} s_{1+n} & -s_n \\ s_n & s_{1-n} \end{bmatrix} \quad \Lambda \equiv \Lambda^1 \quad (173)$$

and use (170) to prove

$$\Lambda^a \Lambda^b = \Lambda^{a+b}. \quad (174)$$

If we write

$$\mathbf{X}_n \equiv \begin{bmatrix} x_{n+1} \\ x_n \end{bmatrix} \quad \mathbf{J}_n \equiv \begin{bmatrix} \frac{T}{\beta} j_n \\ 0 \end{bmatrix} \quad (175)$$

then (166) may be written in the form

$$\mathbf{X}_n = \Lambda \mathbf{X}_{n-1} + \mathbf{J}_n. \quad (176)$$

This equation may be readily solved using the properties of the  $s_a$  functions and by diagonalizing the matrix  $\Lambda$ . We choose Feynman boundary conditions, specifying the particle to be at position  $x_M$  in the past (at time  $MT$ ) and at position  $x_N$  in the future (at time  $NT$ ), giving

$$s s_{N-M} x_n = s s_{N-n} x_M + s s_{n-M} x_N + \frac{T}{\beta} \left\{ \sum_{m=M}^{n-1} s_{N-n} s_{M-m} j_m + s_{N-n} s_{M-n} j_n + \sum_{m=1+n}^N s_{M-n} s_{N-m} j_m \right\} \quad (177)$$

which is valid only for  $M < n < N$ . This can be tidied up into the form

$$x_n = \frac{s_{N-n} x_M}{s_{N-M}} + \frac{s_{M-n} x_N}{s_{M-N}} - T \sum_{m=M}^N G_{NM}^{nm} j_m \quad (178)$$

where

$$\begin{aligned} G_{NM}^{nm} &= -\frac{s_{N-n}s_{M-m}}{\beta s s_{N-M}} & M \leq m < n < N \\ &= -\frac{s_{N-n}s_{M-m}}{\beta s s_{N-M}} & M < m = n < N \\ &= -\frac{s_{M-n}s_{N-m}}{\beta s s_{N-M}} & M < n < m \leq N. \end{aligned} \quad (179)$$

Then  $G_{NM}^{nm}$  satisfies the inhomogeneous equation

$$\beta(U_n - 2\eta + U_n^{-1})G_{NM}^{nm} = -\delta_{n-m} \quad M < n < N. \quad (180)$$

Up to this stage we have taken  $N > M$  with both finite, but normally we will be interested in the scattering limit  $N \rightarrow +\infty$ ,  $M \rightarrow -\infty$ . Also, we have appeared to have overlooked the possibility that  $s_{N-M}$  vanishes in the denominator of the propagator (179) for some values of  $N$  and  $M$ . We shall now address both of these issues directly.

Our method of avoiding possible singularities is to extend the Feynman  $-i\epsilon$  prescription to the  $\theta$  parameter. By inspection of the equation

$$\eta \equiv \cos(\theta) = \frac{6 - 2T^2\omega^2}{6 + T^2\omega^2} \quad (181)$$

we deduce that

$$\omega^2 \rightarrow \omega^2 - i\epsilon \Rightarrow \theta \rightarrow \theta - i\epsilon \quad \eta \rightarrow \eta + i\epsilon. \quad (182)$$

With this deformation of the  $\theta$  parameter and taking the limit  $N \rightarrow +\infty$ ,  $M \rightarrow -\infty$ , we find

$$x_n = \tilde{x}_n - T \sum_{m=-\infty}^{\infty} G_F^{n-m} j_m \quad (183)$$

where  $\tilde{x}_n$  satisfies the homogeneous equation

$$(U_n - 2\eta + U_n^{-1})\tilde{x}_n = 0 \quad (184)$$

and

$$G_F^{n-m} = \frac{1}{2\beta i s} (e^{i(m-n)\theta} \Theta_{n-m} + \delta_{m-n} + e^{i(n-m)\theta} \Theta_{m-n}). \quad (185)$$

This is the discrete time analogue of the harmonic oscillator Feynman propagator and reduces to it in the limit  $T \rightarrow 0$ ,  $nT \rightarrow t$ . A direct application of the discrete time Schwinger action principle to the operator equation of motion

$$(U_n - 2\eta + U_n^{-1})\hat{x}_n = \frac{T}{\beta} j_n \quad (186)$$

then gives the ground state vacuum functional

$$Z[j] = Z[0] \exp \left\{ \frac{-iT^2}{2\hbar} \sum_{n,m=-\infty}^{\infty} j_n G_F^{n-m} j_m \right\} \quad (187)$$

essentially solving the quantum problem. Using this result and (160) we find that in the limit  $j \rightarrow 0$

$$\langle 0 | \hat{x}_n \hat{x}_n | 0 \rangle = \frac{\hbar}{2\beta s} \quad \langle 0 | \hat{x}_{n+1} \hat{x}_n | 0 \rangle = \frac{\hbar}{2\beta s} e^{-i\theta}. \quad (188)$$

From this we deduce

$$\langle 0 | [\hat{x}_{n+1}, \hat{x}_n] | 0 \rangle = \frac{-i\hbar}{\beta} \tag{189}$$

which agrees exactly with the discrete time oscillator commutation relation

$$[\hat{x}_{n+1}, \hat{x}_n] = \frac{-i\hbar}{\beta} \tag{190}$$

found previously.

Further ground-state expectation values of commutators may be obtained by using the result

$$\langle 0 | \tilde{T} \hat{x}_m \hat{x}_n | 0 \rangle = i\hbar G_F^{n-m} = \frac{\hbar}{2\beta \sin \theta} e^{-i|n-m|\theta}. \tag{191}$$

For example, we find

$$\langle 0 | [\hat{x}_{n+2}, \hat{x}_n] | 0 \rangle = \frac{-2i\hbar\eta}{\beta} \tag{192}$$

which agrees with the commutator

$$[\hat{x}_{n+2}, \hat{x}_n] = \frac{-2i\hbar\eta}{\beta} \tag{193}$$

obtained from the operator equation of motion (149) and the commutator (190).

Another verification of the consistency of our methods is that we may use (188) directly to find the ground-state expectation value of the Logan invariant (145) for the discrete time harmonic oscillator. We find

$$\langle 0 | \hat{C}^n | 0 \rangle = \frac{1}{2} \hbar \sqrt{1 - \eta^2} \tag{194}$$

which agrees exactly with previous results.

### 11.2. The hyperbolic regime

Because  $T\omega$  is real and positive the controlling parameter,  $\eta$ , as given by (181) takes values only in the regions

$$\begin{aligned} \text{elliptic:} & \quad -1 < \eta < 1: & \quad 0 < T\omega < 2\sqrt{3} \\ \text{parabolic:} & \quad \eta = -1: & \quad T\omega = 2\sqrt{3} \\ \text{hyperbolic:} & \quad -\infty < \eta < -1: & \quad 2\sqrt{3} < T\omega. \end{aligned} \tag{195}$$

If we parametrize  $\eta$  by the rule  $\eta = \cos(z)$  where  $z$  is complex then if we take

$$\begin{aligned} \eta = \cos \theta: & \quad 0 < T\omega < 2\sqrt{3} \\ \eta = -\cosh \lambda: & \quad 2\sqrt{3} < T\omega \end{aligned} \tag{196}$$

then the range of possibilities (195) corresponds to a contour,  $\Gamma$ , in the complex  $z = \theta - i\lambda$  plane which runs just below the real axis from the origin to  $\pi$  and then runs from  $\pi$  to  $\pi - i\infty$ . The elliptic regime corresponds to values of  $z$  on the first part of the contour, for which  $\lambda = 0 + \epsilon$ , where  $\epsilon$  is infinitesimal and positive, corresponding to the Feynman  $-i\epsilon$  prescription.

The hyperbolic region corresponds to the part of the contour given by  $z = \pi - i\lambda$ ,  $\lambda > 0$ . For this region analytic continuation of the  $s_n$  functions leads to

$$s_n \rightarrow i(-1)^{n+1} \tilde{s}_n \tag{197}$$

where  $\tilde{s}_n \equiv \sinh(n\lambda)$ . From this the analytic continuation of the finite interval propagator (179) gives

$$\tilde{G}_{NM}^{nm} \equiv \frac{-(-)^{n-m}}{\beta\tilde{s}_{N-M}} \{\tilde{s}_{N-n}\tilde{s}_{M-m}\Theta_{n-m} + \tilde{s}_{N-m}\tilde{s}_{M-m}\delta_{n-m} + \Theta_{m-n}\tilde{s}_{M-n}\tilde{s}_{N-m}\} \\ M < n, m < N \quad (198)$$

which satisfies the equation

$$\beta\{U_n - 2\eta + U_n^{-1}\}\tilde{G}_{NM}^{nm} = -\delta_{n-m}. \quad (199)$$

Taking the limit  $N = -M \rightarrow \infty$  gives the infinite interval propagator

$$\tilde{G}_F^{n-m} \equiv \frac{(-)^{1+n-m}}{2\beta\tilde{s}} \{e^{(m-n)\lambda}\Theta_{n-m} + \delta_{n-m} + e^{(n-m)\lambda}\Theta_{m-n}\} \quad (200)$$

which satisfies the equation

$$\beta\{U_n - 2\eta + U_n^{-1}\}\tilde{G}_F^{n-m} = -\delta_{n-m}. \quad (201)$$

### 11.3. Comment

The elliptic and hyperbolic Feynman boundary condition propagators can be summarized in the analytic form

$$\Delta_F^n(\eta) = \frac{T(2 + \cos z)}{6mi \sin z} e^{-i|n|z} \\ = \frac{T(2 + \cos z)}{6mi \sin z} (e^{-inz}\Theta_n + \delta_n + e^{inz}\Theta_{-n}) \quad (202)$$

where  $\eta = \cos z$  and  $z$  lies somewhere on the contour  $\Gamma$  discussed above. Then  $\Delta_F^n(\eta)$  satisfies the equation

$$\beta\{U_n - 2\eta + U_n^{-1}\}\Delta_F^n(\eta) = -\delta_n. \quad (203)$$

However, physical states correspond only to points in the elliptic regime, as the wavefunctions will not remain normalizable in time otherwise. For example, we have previously shown that the ground-state wavefunction for the discrete time oscillator in the elliptic regime is given by

$$\Psi_0(x) = \Psi_0(0) \exp\left(-\frac{1}{2}\beta\sqrt{1-\eta^2}x^2/\hbar\right) \quad (204)$$

demonstrating that analytic continuation to the hyperbolic regime will not give a normalizable ground-state wavefunction.

## 12. Concluding remarks

In this paper we have shown that a consistent approach to the discretization of time results in a consistent dynamical framework. Once the initial psychological hurdle of accepting a dynamics without time derivatives has been jumped, then such a theory becomes as reasonable as continuous time dynamics. Indeed, by taking the fundamental time interval,  $T$ , small enough, it would appear possible to duplicate or approximate conventional theory as closely as required. The obvious question, *why consider discrete time mechanics at all?* has two answers. First, it may be the case after all that there is some fundamental limit to time intervals, and so it becomes a matter of curiosity as to how far we can go along that road. Secondly, there may be some novel properties in this approach which could prevent or

alleviate the notorious problems with divergences which plague conventional field theories. It is worth considering any approach to the regularization in field theory which is based on just one assumption, namely that of a discrete time. The behaviour of the discrete time oscillator holds the promise of potentially useful properties which may provide a cut-off for particle energy.

In the next paper we apply our methods to classical field theories. However, no divergence problems appear at that stage. In the third paper of this series, we shall consider second quantization, and issues concerning divergences of Feynman diagrams will be discussed in subsequent papers in some detail.

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