

# Path integrals, complex probabilities and the discrete Weyl representation\*

W. N. Polyzou

*Department of Physics and Astronomy*

*The University of Iowa*

*Iowa City, IA 52242, USA*

## Abstract

A discrete formulation of the real-time path integral as the expectation value of a functional of paths with respect to a complex probability on a sample space of discrete valued paths is explored. The formulation in terms of complex probabilities is motivated by a recent reinterpretation of the real-time path integral as the expectation value of a potential functional with respect to a complex probability distribution on cylinder sets of paths. The discrete formulation in this work is based on a discrete version of Weyl algebra that can be applied to any observable with a finite number of outcomes. The origin of the complex probability in this work is the completeness relation. In the discrete formulation the complex probability exactly factors into products of conditional probabilities and exact unitarity is maintained at each level of approximation. The approximation of infinite dimensional quantum systems by discrete systems is discussed. The method is illustrated by applying it to scattering theory and quantum field theory. The implications of these applications for quantum computing is discussed.

---

\*This work supported by the U.S. Department of Energy, Office of Science, Grant #DE-SC16457

## I. INTRODUCTION

Quantum computing has become a topic of current research because of its potential for solving problems that are not accessible using digital computers. Quantum computations involve preparing an initial state, evolving it in real time, and performing a measurement at a later time; repeating this for a statistically significant number of measurements. An important step in this process is evolving the prepared initial state using real-time evolution. Real-time path integrals represent unitary time evolution as an integral over a functional of classical paths.

Path integrals are formally derived using the Trotter product formula [1], which expresses real-time evolution as the limit of a product of time evolution over small time steps, making approximations that preserve unitarity and become exact in the limit of small time steps. These are the same steps that quantum computing algorithms are designed to replicate. Real quantum computers are discrete quantum systems with a finite number of qubits. Path integral treatments of real-time evolution in discrete systems can be interpreted as models of quantum computers.

Feynman's interpretation of time evolution as an integral over paths follows by inserting integrals over complete sets of intermediate states at each time step and performing integrals over the intermediate momentum variables. What remains is the limit of products finite-dimensional Fresnel integrals that are interpreted as integrals of a functional of classical paths. This interpretation has great intuitive appeal and is useful for generating perturbative expansions and other results. There are well-known difficulties with the interpretation of time evolution as an integral over paths. The integrand involves oscillations that are not absolutely integrable, and the volume element involves an infinite product of complex quantities. In addition the "action" functional that appears in the integrand has finite difference approximations of derivatives of the paths, where  $\Delta x$  does not get small as  $\Delta t \rightarrow 0$ . The problem with the integral interpretation of the path integral is that there is no positive countably additive measure on the space on paths. This is only a problem with interpretation since the Trotter limit exists independent of the absence of an interpretation as an integral over paths.

An alternative interpretation [2][3][4] was recently introduced that replaces the integral over paths by the expectation value of a functional of paths with respect to a complex

probability on cylinder sets of paths. The concept of complex probabilities is neither intuitive or familiar, however in the Euclidean (imaginary time) case there is a path measure which can alternatively be interpreted as a probability measure. When imaginary-time evolution is replaced by real-time evolution there is no countably additive positive measure on the space of paths and the probabilities become complex. The result of [2][3][4] is that by replacing Lebesgue integration over intermediate states by Henstock [5][6] integration, which can be used to treat products of the Fresnel integrals, it is possible to make mathematical sense of the complex probability interpretation, which results in a global solution of the Schrödinger equation and a unitary one-parameter time-evolution group. This provides a rigorous reinterpretation of real-time path integrals as an average over a collection of classical paths, as suggested by Feynman.

In the real-time case the Gaussian integrals over momenta are replaced by Fresnel integrals which are not absolutely integrable. The Henstock integral is an adaptive generalization of the Riemann integral that performs the cancellation of oscillating quantities in Fresnel integrals before adding them, resulting in finite integrals. For Gaussian Fresnel integrals the Henstock integral gives the same result that is obtained using contour integration. When used in real-time path integrals the integrals over the intermediate spatial coordinates are approximated by the generalized Riemann sums, and paths that have values in sequences of these intervals at different time slices define the cylinder sets of paths. In this interpretation a complex probability is associated with free time evolution of the paths in each cylinder set. The resulting complex probability has most of the properties of a real probability, except that it is not positive and countable additivity is replaced finite additivity.

The purpose of this paper is to further explore application based on the complex probability interpretation of the path integral. While reference [7] was focused on quantum systems that act on infinite dimensional Hilbert spaces, this work develops the complex probability interpretation on finite ( $M$ ) dimensional Hilbert spaces. The finite dimensional case is more closely related to quantum algorithms. In the finite dimensional case the complex probabilities exactly factor into products of conditional probabilities at each time step. Paths are identified with ordered sequences of discrete eigenvalues of quantum observables at different intermediate times. This has the property that there are a finite number of cylinder sets associated with a finite sequence of time slices. An alternative quantum mechanical interpretation is to treat the sequence of eigenvalues as labels for an ordered sequence of

quantum mechanical transition probability amplitudes that result from the dynamics between each time step. The complex probabilities used in this application are due to the completeness sums over intermediate states. Systems with continuous degrees of freedom, which are treated in [7], can be approximated as limits of discrete systems.

Below is a brief outline of the structure of this paper. The ultimate goal is to illustrate by example how discrete methods can in principle be used to perform calculations of scattering observables and the dynamics of quantum fields on a quantum computer. The approach of this work is bottom up in the sense that the continuum dynamics is treated as the limiting case of a sequence of discrete models. Real time evolution of systems on finite dimensional Hilbert spaces is formulated using a path integral representation. Even for these finite dimensional systems there is no countably additive positive measure on the space of paths. In order to address this situation and retain the interpretation of the dynamics as an average over a space of paths, the formal path integral is replaced by the expectation value of a “potential functional” of paths with respect to a complex probability distribution on cylinder sets of paths. This reinterpretation of the path integral was developed in [2][3][4]. In the continuum case complex probability densities are related to products of free particle transfer matrices. While the Fresnel integrals that appear in these transfer matrices are not Riemann integrable, they can be computed using an adaptive generalization of the Riemann integral due to Henstock, which is used to define the complex probabilities. The advantage of the application to discrete systems is that the Fresnel integrals are replaced by finite sums. Since the complex probabilities play a prominent role in this work, their essential properties are discussed briefly in the next section. The general treatment of discrete systems is in discussed in section three. The starting point is a general observable with a finite number of outcomes. It is used, following a method due to Schwinger, to construct an irreducible pair of unitary operators; one commuting with the original observable and one complementary operator with the property that any operator in the Hilbert space can be expressed as a finite degree polynomial in both operators. The path integral representation of the time evolution operator for these discrete systems as the expectation value of a potential functional on cylinder sets of discrete valued paths is developed in section five. The discrete form has the advantage that the complex probability associated with  $N$  time steps exactly factors into a product of conditional probabilities for single time steps. This factorization is used to exactly replace the sum over a large number of paths by powers of a finite dimensional matrix.

While this factorization is already useful, quantum computers are normally formulated on a Hilbert space that is generated by tensor products of qubits. After a short discussion contrasting the difference between classical and quantum computers, the formulation of the discrete path integral in section five is expressed in terms of qubits. This is achieved by starting with an observable on a  $N = 2^L$  dimensional Hilbert space. The irreducible pair of unitary operators is expressed in terms of a collection of  $L$  pairs of complementary unitary operators that act on individual qubits. The elementary unitary operators can be identified with standard quantum gates.

Most problems of interest for quantum computing, like scattering and the dynamics of quantum fields, involve operators with a continuous rather than discrete spectrum. The approximation of the of quantum systems on infinite dimensional Hilbert spaces is treated as the limit of finite dimensional systems discussed in sections five and seven. The resulting formulation of the real-time path integral is given in section eight. The application to a simple model of a particle scattering off of a repulsive Gaussian potential is discussed in the first appendix. The calculations utilize time-dependent methods which involve strong limits. Narrow wave packets in momentum are used to extract sharp momentum transition matrix elements. The second appendix develops the application of these methods to local field theories. For field theories an additional discretization is needed for computations. In this appendix a wavelet basis is used to represent the field in terms of an infinite number of discrete modes. The wavelet representation is an exact representation of the field that replaces fields as operator valued distributions by an infinite collection of well-defined, almost local, canonically conjugate pairs of operators. In this representation singular products of fields are replaced by infinite sums of products of well-defined operators. The representation has natural volume and resolution truncations. Computations require truncations to a finite number of degrees of freedom. The discrete path integral methods are used to compute the time evolution of a  $\phi^4(x)$  field with a Hamiltonian truncated to two modes. While this is a drastic truncation, it illustrates how these discrete methods can be used to model the dynamics of fields.

## II. COMPLEX PROBABILITIES

A complex probability system is defined by a sample set  $S$  and a complex valued function  $P$  on subsets of  $S$  with the properties

$$P(S) = 1. \quad (1)$$

$$P(S_i) + P(S_i^c) = 1 \quad (2)$$

where  $P(S_i)$  is the complex probability assigned to the subset  $S_i$  of  $S$  and  $S_i^c$  is the complement of  $S_i$  in  $S$ . For a finite set of non-intersecting subsets of  $S$

$$S_i \cap S_j = \emptyset, \quad i \neq j \quad P(\cup S_i) = \sum_i P(S_i). \quad (3)$$

In the applications that follow the sample set will be a collection of “paths” that take on discrete values at different times. The relevant subsets  $S_i$  are the sets of paths whose values take on specific discrete values at finite collections of times between 0 and  $t$ . Since  $P(S_i)$  is complex, equation (3) cannot be extended to countable non-intersecting subsets, which is where complex probabilities differ from ordinary probabilities [8][2].

The extension of the notion of complex probabilities to paths with continuous values based on the Henstock integral [5][6][9], was used in [3][4]. The extension of the integral to continuously infinite dimensional path spaces is discussed in [2].

## III. SCHWINGER’S DISCRETE WEYL ALGEBRA

This section reviews Schwinger’s [10] method of constructing an irreducible algebra of complementary unitary operators for quantum systems of a finite number of degrees of freedom. This construction generates a finite degree of freedom version of the Weyl (exponential) form of the canonical commutations relations. This algebra can be used to build discrete models of any finite quantum system.

Let  $X$  be a quantum observable with  $M$  orthonormal eigenvectors  $|m\rangle$  associated with measurement outcomes  $x_m$ .  $X$  acts on an  $M$  dimensional complex Hilbert space  $\mathcal{H}$ . The eigenvectors of  $X$  are a basis on  $\mathcal{H}$ : :

$$X|m\rangle = x_m|m\rangle \quad m = 1, \dots, M. \quad (4)$$

Schwinger defines a unitary operator  $U$  on  $\mathcal{H}$  that cyclically shifts the eigenvectors of  $X$ :

$$U|m\rangle = |m+1\rangle \quad m < M \quad U|M\rangle = |1\rangle. \quad (5)$$

The labels  $m$  on the eigenvectors are treated as integers mod  $M$  so 0 is identified with  $M$ , 1 with  $M+1$  etc.. Since  $M$  applications of  $U$  leaves all  $M$  basis vectors,  $|m\rangle$ , unchanged, it follows that  $U^M = I$ . Since  $U^k|m\rangle$  are independent for all  $k < M$ , there are no lower degree polynomials in  $U$  that vanish, so  $P(\lambda) = \lambda^M - 1 = 0$  is the characteristic polynomial of  $U$ . The eigenvalues  $\lambda$  of  $U$  are the  $M$  roots of 1:

$$\lambda = u_m = e^{\frac{2\pi mi}{M}} \quad (6)$$

with orthonormal eigenvectors  $|u_m\rangle$ :

$$U|u_m\rangle = u_m|u_m\rangle \quad (7)$$

$$\langle u_m|u_n\rangle = \delta_{mn}. \quad (8)$$

The normalization (8) does not fix the phase of the  $|u_n\rangle$  which will be chosen later. Both  $U^M = I$  and  $u_n^M = 1$  imply that

$$\begin{aligned} 0 &= (U^M - I) = \frac{1}{u_n^M}(U^M - I) = \left(\frac{U}{u_n}\right)^M - I = \\ &= \left(\frac{U}{u_n} - I\right)\left(I + \frac{U}{u_n} + \left(\frac{U}{u_n}\right)^2 + \dots + \left(\frac{U}{u_n}\right)^{M-1}\right). \end{aligned} \quad (9)$$

Since this expression is identically zero and  $(\frac{u_m}{u_n} - 1) \neq 0$  for  $m \neq n$  it follows that

$$I + \frac{U}{u_n} + \left(\frac{U}{u_n}\right)^2 + \dots + \left(\frac{U}{u_n}\right)^{M-1} = c|u_n\rangle\langle u_n| \quad (10)$$

for some constant  $c$ . Applying (10) to  $|u_n\rangle$  implies that the constant  $c = M$ . This results in an expression for the projection operator on each eigenstate of  $U$  as a degree  $M-1$  polynomial in  $U$

$$|u_n\rangle\langle u_n| = \frac{1}{M} \sum_{m=1}^M \left(\frac{U}{u_n}\right)^m = \frac{1}{M} \sum_{m=0}^{M-1} \left(\frac{U}{u_n}\right)^m. \quad (11)$$

Using (11) it follows that

$$\begin{aligned} \langle k|u_n\rangle\langle u_n|k\rangle &= \\ \frac{1}{M} \sum_{m=0}^{M-1} \langle k|\left(\frac{U}{u_n}\right)^m|k\rangle &= \end{aligned}$$

$$\begin{aligned} \frac{1}{M} \sum_{m=0}^{M-1} \left(\frac{1}{u_n}\right)^m \langle k|k+m\rangle \\ = \frac{1}{M}. \end{aligned} \quad (12)$$

This means that for any  $k$  and  $n$  that

$$|\langle k|u_n\rangle| = \frac{1}{\sqrt{M}}. \quad (13)$$

The interpretation is that if the system is prepared in any eigenstate of  $U$  and  $X$  is subsequently measured, then the probability of measuring any of the eigenvalues of  $X$  is the same,  $(1/M)$ . This means that all of the information about the identity of the initial eigenstate of  $U$  is lost after measuring  $X$ . This is the condition for the observables  $X$  and  $U$  to be complementary.

It is convenient to choose the phase of each  $|u_n\rangle$  by

$$\langle M|u_n\rangle = \langle u_n|M\rangle = \frac{1}{\sqrt{M}}. \quad (14)$$

It follows from (14) and (11) that

$$\begin{aligned} \langle k|u_n\rangle \langle u_n|M\rangle &= \langle k|u_n\rangle \frac{1}{\sqrt{M}} = \\ \frac{1}{M} \langle k| \sum_{m=1}^M u_n^{-m} |m\rangle &= \frac{1}{M} u_n^{-k} = \\ \frac{1}{M} e^{-2\pi i n k / M}. \end{aligned} \quad (15)$$

Multiplying (15) by  $\sqrt{M}$  shows that the phase convention (14) fixes the inner product  $\langle k|u_n\rangle$  for all  $k \neq M$ :

$$\langle k|u_n\rangle = \frac{1}{\sqrt{M}} e^{-2\pi i n k / M}. \quad (16)$$

Schwinger defines another unitary operator,  $V$ , that shifts the eigenvectors of  $U$  cyclically, but in the opposite direction

$$V|u_n\rangle = |u_{n-1}\rangle, \quad n \neq 1, \quad V|u_1\rangle = |u_M\rangle. \quad (17)$$

The same methods, with  $U$  replaced by  $V$ , give

$$V^M = I \quad (18)$$



$$V|v_m\rangle = v_m|v_m\rangle \quad v_m = e^{\frac{2\pi im}{M}} \quad (19)$$

$$|v_n\rangle\langle v_n| = \frac{1}{M} \sum_{m=0}^{M-1} \left(\frac{V}{v_n}\right)^m = \frac{1}{M} \sum_{m=1}^M \left(\frac{V}{v_n}\right)^m \quad (20)$$

and for unit normalized  $|v_n\rangle$

$$|\langle u_k|v_n\rangle| = \frac{1}{\sqrt{M}}. \quad (21)$$

It is convenient to choose the phase of  $|v_n\rangle$  by the condition

$$\langle u_M|v_n\rangle = \frac{1}{\sqrt{M}}. \quad (22)$$

then (20) and the orthonormality of the  $|u_k\rangle$ 's give

$$\begin{aligned} \langle u_M|v_n\rangle\langle v_n|u_k\rangle &= \langle v_n|u_k\rangle \frac{1}{\sqrt{M}} = \\ \frac{1}{M} \sum_{m=0}^{M-1} v_n^{-m} \langle u_m|u_k\rangle &= \frac{1}{M} v_n^{-k}. \end{aligned} \quad (23)$$

Multiplying (23) by  $\sqrt{M}$  gives

$$\langle v_k|u_n\rangle = \frac{1}{\sqrt{M}} e^{-2\pi ink/M}. \quad (24)$$

Comparing (16) and (24) it follows that

$$\begin{aligned} |v_k\rangle &= \sum_{m=0}^{M-1} |u_m\rangle \langle u_m|v_k\rangle = \\ &= \sum_{m=0}^{M-1} |u_m\rangle \frac{e^{2\pi imk/M}}{\sqrt{M}} = \\ &= \sum_{m=0}^{M-1} |u_m\rangle \langle u_m|k\rangle = |k\rangle, \end{aligned} \quad (25)$$

so, because of the phase choices, the operators  $X$  and  $V$  have the same eigenvectors.

The spectral expansion of  $V$ , the identification (25) of  $|v_k\rangle$  with  $|k\rangle$  and the definition (5) of  $U$  imply that the unitary operators  $U$  and  $V$  satisfy

$$\begin{aligned} UV &= U \sum_{m=0}^{M-1} |v_m\rangle e^{\frac{i2\pi m}{M}} \langle v_m| = \\ &= \sum_{m=0}^{M-1} |v_{m+1}\rangle e^{\frac{i2\pi m}{M}} \langle v_m| = \sum_{m=0}^{M-1} |v_{m+1}\rangle e^{\frac{i2\pi m}{M}} \langle v_{m+1}| U = \end{aligned}$$

$$\sum_{m=0}^{M-1} |v_{m+1}\rangle e^{\frac{i2\pi(m+1)}{M}} e^{-\frac{2\pi i}{M}} \langle v_{m+1}| U = e^{-\frac{2\pi i}{M}} V U. \quad (26)$$

$U$  and  $V$  generate a complete set of operators in the sense that any operator on the Hilbert space can be expressed as a degree  $(M-1) \times (M-1)$  polynomial these two operators. Note that  $m-k$  applications of (5) give  $U^{m-k}|v_k\rangle = |v_m\rangle$ . Using this with (20) gives

$$\begin{aligned} |v_m\rangle \langle v_k| &= U^{m-k} |v_k\rangle \langle v_k| = \\ &= \frac{1}{M} \sum_{n=0}^{M-1} e^{-2\pi i n k / M} U^{m-k} V^n. \end{aligned} \quad (27)$$

The order of the  $U$  and  $V$  operators can be changed using multiple applications of (26):

$$\begin{aligned} U^m V^n &= U^{m-1} V^n U e^{-\frac{2n\pi i}{M}} = U^{m-2} V^n U^2 e^{-\frac{4n\pi i}{M}} = \\ &\dots = V^n U^m e^{-\frac{2mn\pi i}{M}}. \end{aligned} \quad (28)$$

Using (28) in (27) gives

$$\begin{aligned} |v_m\rangle \langle v_k| &= \\ &= \frac{1}{M} \sum_{n=0}^{M-1} e^{-2\pi i n k / M} V^n U^{m-k} e^{-\frac{2(m-k)n\pi i}{M}} = \\ &= \frac{1}{M} \sum_{n=0}^{M-1} e^{-2\pi i n k / M} V^n U^{m-k}. \end{aligned} \quad (29)$$

A general operator  $O$  can be expressed in terms of its matrix elements in a basis

$$\begin{aligned} O &= \sum_{m,k=0}^{M-1} |v_m\rangle \langle v_m| O |v_k\rangle \langle v_k| = \\ &= \sum_{m,k=0}^{M-1} \langle v_m| O |v_k\rangle |v_m\rangle \langle v_k| = \\ &= \frac{1}{M} \sum_{m,n,k=0}^{M-1} e^{-2\pi i n k / M} \langle v_m| O |v_k\rangle U^{m-k} V^n = \\ &= \frac{1}{M} \sum_{m,n,k=0}^{M-1} e^{-2\pi i m n / M} \langle v_m| O |v_k\rangle V^n U^{m-k}. \end{aligned} \quad (30)$$

These equations have the form

$$O = \sum_{m,n=0}^{M-1} c_{mn} U^m V^n = \sum_{m,n=0}^{M-1} d_{mn} V^m U^n \quad (31)$$

which is the discrete Weyl representation of  $O$ . If  $O$  commutes with  $U$  then, using (28),

$$0 = \sum_{mn=0}^{M-1} c_{mn} [U^m V^n, U] = \sum_{mn=0}^{M-1} c_{mn} U^{m+1} V^n (e^{2\pi i n/M} - 1) \quad (32)$$

which requires  $n = M$  or  $0$ . This means  $O$  is independent of  $V$ . Similarly if  $O$  commutes with  $V$  it must be independent of  $U$ . It follows that any operator that commutes with both  $U$  and  $V$  is a constant multiple of the identity. This means that the operators  $U$  and  $V$  are an irreducible set of unitary operators.

#### IV. PATH INTEGRALS FOR FINITE DIMENSIONAL SYSTEMS

This section considers a general system of a finite number,  $M$ , of degrees of freedom.  $X$  is the observable of interest. It evolves under the influence of a Hamiltonian  $H$  which is a Hermitian matrix on the  $M$ -dimensional Hilbert space. A measurement of  $X$  gives one of its eigenvalues,  $x_n$ . The  $M$  eigenvectors of  $X$  are chosen to be orthonormal. The notation,  $|n\rangle$ ,  $1 \leq n \leq M$  is used to label these eigenvectors.  $X$  is analogous to a ‘‘coordinate’’ operator in this setting, but in principle it can be any Hermitian operator on  $\mathcal{H}$ .

The quantity of interest is the probability amplitude for a transition from an initial eigenstate of  $|n_i\rangle$  of  $X$  to a final eigenstate  $|n_f\rangle$  after time  $t$ . This is given by the matrix element of the unitary time evolution operator

$$\langle n_f | e^{-iHt} | n_i \rangle. \quad (33)$$

In this section (33) is expressed as the expectation value of a ‘‘functional of paths’’ with respect to a complex probability on a space of paths.

Following the construction in the previous section irreducible pairs of unitary operators  $U$  and  $V$  can be constructed from  $X$ . The eigenvectors  $|n\rangle$  of  $V$  are identical to the eigenvectors of  $X$ , while the eigenvectors  $|\bar{m}\rangle$  of  $U$  are complementary in the sense that

$$|\langle u | \bar{m} \rangle|^2 = \frac{1}{M}. \quad (34)$$

$U$  satisfies

$$U|n\rangle = |n+1\rangle \quad U|\bar{n}\rangle = |\bar{n}\rangle e^{i\frac{2\pi n}{M}}, \quad (35)$$

$V$  satisfies

$$V|\bar{n}\rangle = |\bar{n}-1\rangle \quad V|n\rangle = |n\rangle e^{i\frac{2\pi n}{M}} \quad (36)$$

and

$$VU = UV e^{i\frac{2\pi}{M}}. \quad (37)$$

The inner product of the eigenvectors of these complementary operators is

$$\langle n|\bar{m}\rangle = \frac{e^{-imn\phi}}{\sqrt{M}}. \quad (38)$$

The time-evolution operator can be expressed as the  $N^{\text{th}}$  power of a unitary transfer matrix  $T$ :

$$e^{-iHt} = T^N \quad T = e^{-iH\Delta t} \quad \text{where} \quad \Delta t = t/N. \quad (39)$$

Since the pair of operators  $U$  and  $V$  is irreducible,  $T$  or  $H$  can be expressed as degree  $(M-1) \times (M-1)$  polynomials in  $U$  and  $V$  using (31):

$$T = \sum_{mn} t_{mn} U^m V^n \quad H = \sum_{mn} h_{mn} U^m V^n. \quad (40)$$

The quantities  $t_{mn}$  and  $h_{mn}$  are complex valued functions of two discrete variables. The eigenvalues of  $X$  can be taken as one of the variables. It is useful to define another Hermitian operator  $P$  that has the same eigenvectors as  $U$  with eigenvalues  $p_n$  analogous to the relation between  $X$  and  $V$ :

$$P|\bar{m}\rangle = p_m|\bar{m}\rangle. \quad (41)$$

The eigenvalues  $x_n$  and  $p_m$  will be referred to as ‘‘coordinates’’ and ‘‘momenta’’ for the purpose of illustration, although in general they have no relation to coordinates and momenta. In this section the choice of the eigenvalues,  $p_m$ , is not important - all that is used are the eigenvectors,  $|\bar{m}\rangle$ . Matrix elements of the transfer matrix in a mixed  $(x, p)$  basis can be computed using (35), (36) in (40):

$$\langle \bar{n}|T|m\rangle = \langle \bar{n}|m\rangle \tilde{T}_{nm} \quad (42)$$

where the numerical coefficients  $\tilde{T}_{nm}$  are

$$\tilde{T}_{nm} = \sum_{kl} t_{kl} e^{-2\pi i \frac{(nk-ml)}{M}}. \quad (43)$$

Mixed matrix elements of the Hamiltonian have a similar form

$$\langle \bar{n} | H | m \rangle = \langle \bar{n} | m \rangle \tilde{H}_{nm} \quad \tilde{H}_{nm} = \sum_{kl} h_{kl} e^{-2\pi i \frac{(nk-ml)}{M}}. \quad (44)$$

Changing the “momentum”  $|\bar{n}\rangle$  basis back to the “coordinate”  $|n\rangle$  basis gives

$$\langle k | T | m \rangle = \sum_n \langle k | \bar{n} \rangle \langle \bar{n} | m \rangle \tilde{T}_{nm} \quad (45)$$

and

$$\langle k | H | m \rangle = \sum_n \langle k | \bar{n} \rangle \langle \bar{n} | m \rangle \tilde{H}_{nm}. \quad (46)$$

Matrix elements of the time evolution operator in the coordinate basis can be expressed, using representation (45-46) in (39), as

$$\begin{aligned} \langle k_f | e^{-iHt} | k_i \rangle &= \langle k_f | [e^{-iHt/N}]^N | k_i \rangle = \\ &= \sum_{k_1 \cdots k_N} \langle k_f | T | k_N \rangle \langle k_N | T | k_{N-1} \rangle \cdots \langle k_2 | T | k_1 \rangle \langle k_1 | T | k_i \rangle = \\ &= \sum_{k_1 \cdots k_N} \langle k_f | \bar{n}_N \rangle \langle \bar{n}_N | k_N \rangle \langle k_N | \bar{n}_{N-1} \rangle \langle \bar{n}_{N-1} | k_{N-1} \rangle \cdots \\ &\quad \langle k_3 | \bar{n}_2 \rangle \langle \bar{n}_2 | k_2 \rangle \langle k_2 | \bar{n}_1 \rangle \langle \bar{n}_1 | k_i \rangle \times \\ &\quad \tilde{T}_{n_N k_N} \tilde{T}_{n_{N-1} k_{N-1}} \cdots \tilde{T}_{n_2 k_2} \tilde{T}_{n_1 k_i}. \end{aligned} \quad (47)$$

The time step,  $t/N$ , appears in the coefficients  $\tilde{T}_{n_m k_m}$ . These are complex numbers.

If the  $\tilde{T}_{n_m k_m}$  are all set to 1 then what remains after performing the completeness sums is the overlap of the final “coordinate” with the initial “coordinate”,  $\langle k_f | k_i \rangle = \delta_{k_f, k_i}$ . An additional sum over  $k_i$  (resp  $k_f$ ) or gives 1, independent of  $k_f$  (resp  $k_i$ ). This motivates the definition of the complex probability

$$\begin{aligned} P_N(k_f; n_N, k_N, \cdots n_1, k_1) &:= \\ &= \langle k_f | \bar{n}_N \rangle \langle \bar{n}_N | k_N \rangle \langle k_N | \bar{n}_{N-1} \rangle \langle \bar{n}_{N-1} | k_{N-1} \rangle \\ &\quad \vdots \\ &= \langle k_3 | \bar{n}_2 \rangle \langle \bar{n}_2 | k_2 \rangle \langle k_2 | \bar{n}_1 \rangle \langle \bar{n}_1 | k_1 \rangle \end{aligned} \quad (48)$$

which by completeness satisfies

$$\sum_{n_1, k_1 \cdots n_N, k_N} P_N(k_f; n_N, k_N, \cdots n_1, k_1) = 1 \quad (49)$$

for any  $|k_f\rangle$ .  $P_N$  assigns a complex weight to a pair of eigenvalues of  $X$  and  $P$  at each of  $N$  time steps.

The exact time evolution can be expressed using the Trotter product formula

$$e^{-iHt} = \lim_{N \rightarrow \infty} (e^{-iHt/N})^N = \lim_{N \rightarrow \infty} (I - iHt/N)^N$$

where only the first order term in the exponent contributes in the limit  $N \rightarrow \infty$ . In the small  $\Delta t = t/N$  limit

$$\begin{aligned} \langle \bar{m}|T|n\rangle &\approx \langle \bar{m}|I - iH\Delta t|n\rangle = \\ \langle \bar{m}|n\rangle(1 - i\tilde{H}_{mn}\Delta t) &\approx \langle \bar{m}|n\rangle e^{-i\tilde{H}_{mn}\Delta t}. \end{aligned} \quad (50)$$

In this expression  $\tilde{H}_{mn}$  is an ordinary function of  $p_m$  and  $x_n$ . If the quantum Hamiltonian  $H$  is expressed with the  $X$  operators to the right of the  $P$  operators, this would be the Hamiltonian with these operators replaced by the ‘‘coordinates’’ and ‘‘momenta’’. It is the analog of a classical phase space Hamiltonian.

It follows from (42) and (50) that

$$\tilde{T}_{nk} \approx e^{-i\tilde{H}(p_n, x_k)\Delta t}$$

and

$$\tilde{T}_{n_N k_N} \tilde{T}_{n_{N-1} k_{N-1}} \cdots \tilde{T}_{n_2 k_2} \tilde{T}_{n_1 k_1} \approx e^{-i\sum_m \tilde{H}(p_{n_m}, x_{k_m})\Delta t} \quad (51)$$

which is a functional of a classical ‘‘phase space’’ path  $p(t), x(t)$  with endpoints at  $x(0)$  and  $x(t)$ , where  $p(t), x(t)$  can take on  $M$  discrete values,  $p_n$  and  $x_m$  at each time step. This is classical in the sense that even though  $P$  and  $X$  do not commute,  $\tilde{H}(p_n, x_m)$  is an ordinary function of the eigenvalues  $p_n$  and  $x_m$ . A *cylinder set of paths* is a set of  $M$ -valued functions  $p(t)$  and  $x(t)$  that take on one of the  $M$  possible eigenvalues of  $P$  and  $X$  at each of  $N$  time slices, subject to initial and final values of the  $x$  variable. With this definition of cylinder set

$$P_N(k_f; n_N, k_N, \cdots n_1, k_1) \quad (52)$$

can be interpreted as a complex probability associated with the cylinder set of ‘‘phase space’’ paths that start at  $x_{k_1}$ , end at  $x_{k_f}$  and have values  $p_{n_m}, x_{k_m}$  at the  $m^{\text{th}}$  time slice.

From a quantum mechanical point of view an  $M$ -valued path can be thought of as an ordered sequence of quantum transition amplitudes that alternate between states of irreducible pairs of observables.

Combining (47,48 and 50) gives

$$\langle k_f | e^{-iHt} | k_i \rangle \approx \sum_{n_N, k_N, \dots, n_1, k_1} P_N(k_f; n_N, k_N, \dots, n_1, k_1) e^{-i \sum_m \tilde{H}(x_{nm}, p_{k_m}) \Delta t} \delta_{k_1 k_i} \quad (53)$$

which approximates the transition probability amplitude as the expectation value of a functional of the “classical” Hamiltonian  $\tilde{H}(x, p)$  over cylinder sets of “paths in phase space”. Here the “coordinate” paths have fixed endpoints at 0 and  $t$ , while the “momentum” paths are unconstrained. In this case the complex probability interpretation is a consequence of the completeness relation.

In general the number of cylinder sets that must be summed over is prohibitively large, ( $\sim M^{2N}$ ). The definition (48) implies that the complex probability can be factored into products of one-step probabilities

$$P_N(k_f; n_N, k_N, \dots, n_1, k_1) = \prod_{i=1}^N \langle k_{i+1} | \bar{n}_i \rangle \langle \bar{n}_i | k_i \rangle := \prod_i P(k_{i+1}; n_i, k_i), \quad k_{N+1} = k_f. \quad (54)$$

In this case

$$\langle k_f | e^{-iHt} | k_i \rangle = \sum_{n_N, k_N, \dots, n_1, k_1} \prod_i \left( P(k_{i+1}; n_i, k_i) e^{-i \tilde{H}(x_{n_i}, p_{k_i}) \Delta t} \right) \delta_{k_1 k_i} \quad (55)$$

where  $k_{N+1} = k_f$ . This reduces the computation of (53) to computing the  $N^{th}$  power of an  $M \times M$  matrix.

The formalism discussed above can be applied to any Hamiltonian on the  $M$ -dimensional Hilbert space. If the Hamiltonian is a sum of the form  $\tilde{H}(p, x) = \tilde{H}_1(p) + \tilde{H}_2(x)$  then it is possible to sum over the intermediate “momentum” variables resulting in a complex probability on a space of paths in the coordinate variable,  $X$ .

In this case

$$\begin{aligned} \sum_n \langle k | \bar{n} \rangle \langle \bar{n} | H | m \rangle &= \\ \sum_n \langle k | \bar{n} \rangle \langle \bar{n} | m \rangle (H_1(p_n) + H_2(x_m)) &= \\ \sum_n \langle k | \bar{n} \rangle \langle \bar{n} | m \rangle \tilde{H}_{nm} & \end{aligned} \quad (56)$$

where  $\tilde{H}_{nm}$  is just the ‘‘classical’’ Hamiltonian as a function of the eigenvalues.

A new complex probability can be defined by

$$P_X(k_f; k_N, \dots, k_1) := e^{i\tilde{H}_1(p_0)t} \sum_{n_1 \dots n_N} P(k_f; n_N, k_N, \dots, n_1, k_1) e^{-i \sum \tilde{H}_1(p_{nm}) \Delta t}. \quad (57)$$

To show that this is normalized like a complex probability, interchange the order of the sum over the intermediate  $k$  indices and  $n$  indices (both sums are finite). The  $k_2 \dots k_N$  sums are just expressions for the identity. After eliminating  $k_2 \dots k_N$  what remains is a product of Kronecker delta functions in the  $n_i$  variables. Since the operator  $H_1$  is a multiplication operator in the  $n$  variables, all but one of the  $n$  sums can be performed giving:

$$\begin{aligned} \sum_{n_1 \dots n_N} \sum_{k_1 \dots k_N} P(k_f; n_N, k_N, \dots, n_1, k_1) e^{-i \sum \tilde{H}_1(p_{nm}) \Delta t} = \\ \sum_{n=0}^{M-1} \sum_{k_1=0}^{M-1} \langle k_f | \bar{n} \rangle e^{-iN\tilde{H}_1(p_n)\Delta t} \langle \bar{n} | k_1 \rangle. \end{aligned}$$

The  $k_1$  sum can be evaluated using

$$\begin{aligned} \sum_{n=0}^{M-1} \sum_{k_1=0}^{M-1} \langle k_f | \bar{n} \rangle e^{-i\tilde{H}_1(p_n)t} \langle \bar{n} | k_1 \rangle = \\ \frac{1}{M} \sum_{n=0}^{M-1} e^{-i2\pi k_f n/M} \sum_{k_1=0}^{M-1} e^{i2\pi k_1 n/M} e^{-i\tilde{H}_1(p_n)t} = \\ \frac{1}{M} \sum_{n=0}^{M-1} e^{-i2\pi k_f n/M} e^{-i\tilde{H}_1(p_n)t} \times \\ \begin{cases} (1 - e^{i2\pi M n/M}) = 0 & 1 < n < M - 1 \\ M & n = 0 \end{cases} \\ = \delta_{n0} e^{-iH_1(p_0)t}. \end{aligned} \quad (58)$$

Including the factor  $e^{iH_1(p_0)t}$  gives

$$\begin{aligned} \sum_{k_1 \dots k_N} P_X(k_f; k_N, \dots, k_1) = \\ e^{i\tilde{H}_1(p_0)t} \sum_{n=0}^{M-1} \sum_{k_1=0}^{M-1} P(k_f; n_N, k_N, \dots, n_1, k_1) e^{-i \sum_m \tilde{H}_1(p_m) \Delta t} = 1. \end{aligned} \quad (59)$$



The expression for the evolution operator becomes

$$\langle k_f | e^{-iHt} | k_i \rangle = \sum_{k_1 \dots k_N} P_X(k_f; , k_N, \dots, k_1) e^{-i \sum_m \tilde{H}_2(x_{n_m}) \Delta t} \delta_{k_1 k_i} \quad (60)$$

which is expressed as the expectation value of the functional  $e^{-i \sum_m \tilde{H}_2(x_{n_m}) \Delta t}$  on cylinder sets of discrete paths. The finite sums over the discrete intermediate “momentum” variables replace the Gaussian Fresnel integrals in the continuum case.

In this case the complex probability over cylinder sets of paths in  $x$  also factors into products of one-step probabilities with

$$P_X(k_{n+1}; k_n) = \sum_m P(k_{n+1}; m, k_n) e^{-i(\tilde{H}_1(p_m) - \tilde{H}_1(p_0)) \Delta t} \quad (61)$$

giving

$$\langle k_f | e^{-iHt} | k_i \rangle = \lim_{N \rightarrow \infty} \sum \left( \prod_n P_X(k_{n+1}; k_n) e^{-i \sum_m \tilde{H}_2(p_n) \Delta t} \right) \delta_{k_1, k_i} \quad k_f = k_{N+1} \quad (62)$$

which has the structure of the  $N^{\text{th}}$  power of an  $M \times M$  matrix. In this discrete case the result becomes exact in the Trotter limit.

In the discrete case time evolution can be solved exactly by diagonalizing the  $M \times M$  Hamiltonian matrix in the  $x$  basis, however the appeal of the discrete path integral is that it is a model of a quantum circuit. Accuracy can be improved by using a higher order approximation to the transfer matrix at each step. The complex probability interpretation is a natural way to think about real-time path integrals.

The advantage of this approach is that the time evolution is approximated by calculating the expectation value functional of a finite set of “classical” paths with respect to a complex probability distribution. The ability to exactly factor the complex probability into products of one step probabilities for each time step facilitates the computation. Finally exact unitarity is maintained at each step. While the limit for continuous time evolution exists [3][4], real computations are truncated at a finite number of time steps.

## V. QUANTUM LOGIC

The interest in discrete path integrals is that they serve as models of quantum computers. The difference between classical and quantum computers is related to the difference between

classical and quantum logic. Classically if a system is prepared in a state  $A$  and a later measurement tests if it will be detected in state  $B$ , there are two possible outcomes, true or false. This leads to a two valued system of logic that is encoded in the bits used in digital computing. In quantum mechanics there are three possibilities - the final system will always be measured to be in the state  $B$ , it will never be measured to be in the state  $B$ , or there is a finite probability  $P$ , with  $0 < P < 1$ , that it will be measured to be in state  $B$ . This leads to a three-valued logic or quantum logic.

The three valued logic of quantum mechanics [11] has a straightforward geometrical interpretation. If state  $A$  is represented by a one-dimensional subspace of a Hilbert space and state  $B$  is represented by another one-dimensional subspace then there are three possibilities - (1) the subspace  $B$  is the subspace  $A$ , (2) the subspace  $B$  is orthogonal to the subspace  $A$  or (3) any non-0 vector in  $A$  has a non-zero projection on the subspace  $B$ .

In the quantum case states are represented by vectors or rays,  $|a\rangle$  in a Hilbert space. Quantum probabilities are expressed in terms of the Hilbert space inner product:

$$P_{ab} := \frac{\langle a|b\rangle\langle b|a\rangle}{\langle a|a\rangle\langle b|b\rangle} \quad (63)$$

which is independent of the vectors in the rays. The three possibilities correspond to

$$(1)P_{ab} = 1 \quad (64)$$

$$(2)P_{ab} = 0 \quad (65)$$

$$(3)0 < P_{ab} < 1. \quad (66)$$

When the Hilbert space is two dimensional the difference in these two types of logic is encoded in bits or qubits respectively. A bit can only be in one of two states, true or false. For a qubit in a spin up state, the three possibilities are (1) the probability of measuring it to be in a spin up state is 1 (true), (2) the probability of measuring it to be in a spin down state is 0 (false) and (3) the probability of measuring it to be in a non-trivial linear combination up and down states is a positive number strictly between zero and one (maybe).

The discrete path integral developed in the previous section represents the transition probability amplitude as the expectation value of a random variable on a space of sequences of transition amplitudes labeled by paths in the space of eigenvalues of complementary observables.

## VI. QUBITS

One property of Schwinger's discrete Weyl algebra is that it has a natural representation in terms of qubits. When  $M$  can be factored into products of prime numbers the  $U$  and  $V$  operators can be replaced by an algebra of commuting pairs of operators with cycles the length of each prime factor. The case of most interest for quantum computing is when  $M = 2^L$ . In that case the irreducible algebra is represented by tensor products of qubit gates. For systems where the number of degrees of freedom  $K$  is not a power of two, they can be embedded in a space of dimension  $M = 2^L$ , for  $M > K$ .

Consider the case where  $M = 2^L$  for large  $L$ . The indices  $n = 0 \dots 2^L - 1$  can be labeled by  $L$  numbers that can only take the values 0 and 1. It has a L-bit representation  $n \leftrightarrow (n_1, n_2, \dots, n_L)$

$$n = \sum_{m=1}^L n_m 2^{m-1}. \quad (67)$$

This results in the identifications

$$|u_{n_1 \dots n_L}\rangle := |u_n\rangle \quad |v_{n_1 \dots n_L}\rangle := |v_n\rangle. \quad (68)$$

Define unitary operators  $U_i$  and  $V_i$  by

$$U_i |v_{n_1 \dots n_L}\rangle = |v_{n_1 \dots [n_i+1]_{\text{mod } 2} \dots n_L}\rangle \quad (69)$$

$$V_i |u_{n_1 \dots n_L}\rangle = |u_{n_1 \dots [n_i-1]_{\text{mod } 2} \dots n_L}\rangle. \quad (70)$$

Applying what was done in the general case to  $M = 2^L$  gives

$$U_i^2 - 1 = V_i^2 - 1 = 0, \quad (71)$$

$$[U_i, U_j] = [V_i, V_j] = 0 \quad [U_i, V_j] = 0 \quad i \neq j, \quad (72)$$

$$V_i U_i = U_i V_i e^{i\pi}, \quad (73)$$

$$U^n = \prod_{m=1}^L U_m^{n_m}, \quad (74)$$

$$V^n = \prod_{m=1}^L V_m^{n_m}. \quad (75)$$

Since  $U$  and  $V$  can be constructed from the  $U_i$  and  $V_i$  the set of  $\{U_i\}$  and  $\{V_i\}$  is also irreducible.

A matrix representation of  $U_i$  and  $V_i$  acting on the  $i$ -th qubit is

$$V_i = \sigma_3 \quad U_i = \sigma_1 \quad (76)$$

which are simple quantum gates. In this representation,  $v_0 = u_0 = 1; v_1 = u_1 = -1$  and

$$|v_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |v_1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (77)$$

$$|u_0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |u_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \quad (78)$$

The operators  $\sigma_1$  and  $\sigma_3$

$$U_i = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad V_i = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (79)$$

satisfy (5) and (17) for  $M = 2$ . They also satisfy

$$\sigma_3\sigma_1 = \sigma_1\sigma_3 e^{\frac{2\pi i}{2}} \quad (\sigma_1^2 - 1) = (\sigma_3^2 - 1) = 0. \quad (80)$$

Any linear operator  $A$  on this 2-dimensional vector space is a polynomial with constant coefficients  $a_i$  in these operators:

$$A = a_1 I + a_2 \sigma_1 + a_3 \sigma_3 + a_4 \sigma_3 \sigma_1. \quad (81)$$

In this case the Hilbert space is represented by  $L$  qubits. The irreducible set of operators,  $U_i$  and  $V_i$  are represented by  $L$  pairs of Pauli matrices ( $\sigma_1$  and  $\sigma_3$ ) that act on each qubit. This representation has the advantage that it is local in the sense that the  $U_i$  and  $V_i$  operators act on a single qubit and the operators that act on different qubits commute. Equations (74-75) relate the operators that appear in the discrete path integral to tensor products of single qubit operators  $\sigma_1$  and  $\sigma_3$ .

## VII. SCHWINGER'S CONTINUUM LIMIT

While quantum computers are discrete quantum systems, many problems of interest involve observables like momenta, coordinates, and canonical fields that have continuous spectra. Applications require discrete approximations to these continuous systems. It is

possible to use the discrete algebra generated by  $U$  and  $V$  to make a discrete approximation to the continuum in the large  $M$  limit. The limit is designed to give a representation of the Weyl algebra.

For large  $M$  Schwinger [10] defines the small quantity  $\epsilon$  by

$$\epsilon^2 := 2\pi/M. \quad (82)$$

For the purpose of approximating the continuum it is convenient (but not necessary) to choose  $M = 2K + 1$  odd and number the eigenvectors and eigenvalues from  $-K \leq n \leq K$  instead of 0 to  $M-1$  or 1 to  $M$  (For even  $M$  the indices could be labeled  $-M/2 \leq n \leq M/2$ ). Discrete approximations to continuous variables  $p$  and  $x$  are defined by

$$p_l = l\epsilon = l\sqrt{\frac{2\pi}{M}} \quad x_l = l\epsilon = l\sqrt{\frac{2\pi}{M}} \quad -K\epsilon \leq x_l, p_l \leq K\epsilon \quad (83)$$

where

$$K\epsilon = \sqrt{\frac{M\pi}{2}} - \sqrt{\frac{\pi}{2M}}. \quad (84)$$

With these definitions the separation between successive values of  $p_l$  and  $x_l$ ,  $p_{l+1} - p_l = x_{l+1} - x_l = \epsilon$  vanishes as  $M \rightarrow \infty$  while at the same time the maximum and minimum values of  $p_l$  and  $x_l$ ,  $p_{\pm K} = x_{\pm K} = \pm(\sqrt{\frac{M\pi}{2}} - \sqrt{\frac{\pi}{2M}})$  approach  $\pm\infty$  in same limit.

While for finite  $M$  any vector with a finite number of elements has a finite norm, in the continuum limit ( $M \rightarrow \infty$ ) this is no longer true so the limiting vectors with finite norm should be square summable. This means that components of vectors with large  $|l|$  should approach 0 in the  $M \rightarrow \infty$  limit.

For unitary operators  $U$  and  $V$  given by (5) and (18) Hermitian operators  $\tilde{p}$  and  $\tilde{x}$  are defined by

$$V = e^{i\epsilon\tilde{p}} \quad U = e^{i\epsilon\tilde{x}}. \quad (85)$$

These can be used to define

$$V(x_m) = e^{i\tilde{p}x_m} = e^{i\tilde{p}\epsilon m} = V^m \quad (86)$$

$$U(p_n) = e^{i\tilde{x}p_n} = e^{i\tilde{x}\epsilon n} = U^n. \quad (87)$$

With these definitions equation (25) becomes

$$V(x_m)U(p_k) = U(p_k)V(x_m)e^{\frac{i2\pi mk}{M}} =$$

$$U(p_k)V(x_m)e^{i\epsilon m\epsilon k} = U(p_k)V(x_m)e^{ip_k x_m} \quad (88)$$

which is the Weyl [12] form of the canonical commutation relations, where in this case the variables are discrete. In order to take the continuum limit define numbers  $p := \epsilon n$  and  $x = \epsilon m$ . This motivates the definitions

$$dp = \epsilon dn = \sqrt{\frac{2\pi}{M}} dn \quad dx = \epsilon dm = \sqrt{\frac{2\pi}{M}} dm. \quad (89)$$

It follows from (85) that eigenvectors of  $V$  are also eigenvectors of  $\tilde{p}$  and the eigenvectors of  $U$  are also eigenvectors of  $\tilde{x}$ . Choosing the normalization of the states  $|p_n\rangle$  and  $|x_n\rangle$  so

$$\int dp \approx \sum_{n=-K}^K \frac{dp}{dn} = \epsilon \sum_{n=-K}^K \quad (90)$$

$$\int dx \approx \sum_{m=-K}^K \frac{dx}{dm} = \epsilon \sum_{m=-K}^K \quad (91)$$

$$I = \sum_{l=-K}^K |v_l\rangle\langle v_l| = \sum_{l=-K}^K |p_l\rangle dp_l \langle p_l| = \sum_{l=-K}^K |p_l\rangle \epsilon \langle p_l| \quad (92)$$

$$I = \sum_{l=-K}^K |u_l\rangle\langle u_l| = \sum_{l=-K}^K |x_l\rangle dx_l \langle x_l| = \sum_{l=-K}^K |x_l\rangle \epsilon \langle x_l| \quad (93)$$

which expresses the sum over small steps in  $p$  or  $x$  as integrals. Equations (92) and (93) imply the relations

$$|p_l\rangle := |v_l\rangle / \sqrt{\epsilon} \quad (94)$$

and

$$|x_l\rangle := |u_l\rangle / \sqrt{\epsilon}. \quad (95)$$

Using these relations gives

$$\langle p_m | x_n \rangle = \frac{1}{\epsilon} \langle v_m | u_n \rangle = \frac{1}{\epsilon \sqrt{M}} e^{-\frac{2\pi i m n}{M}} = \frac{1}{\sqrt{2\pi}} e^{-ip_m x_n} \quad (96)$$

$$\langle p_m | p_n \rangle = \frac{1}{\epsilon} \langle v_m | v_n \rangle = \frac{\delta_{mn}}{\epsilon} \quad (97)$$

and

$$\langle x_m | x_n \rangle = \frac{1}{\epsilon} \langle u_m | u_n \rangle = \frac{\delta_{mn}}{\epsilon}. \quad (98)$$

In this notation equations (86) and (87) with (5) and (17) give imply

$$U(x_m)|x_n\rangle = |x_m + x_n\rangle \quad (99)$$

$$V(p_m)|p_n\rangle = |p_m - p_n\rangle \quad (100)$$

which can be expressed in terms of the “continuum variables” as

$$U(x)|x'\rangle = |x' + x\rangle \quad (101)$$

$$V(p)|p'\rangle = |p' - p\rangle \quad (102)$$

### VIII. COMPLEX PROBABILITIES IN REAL-TIME PATH INTEGRALS ON INFINITE DIMENSIONAL HILBERT SPACES

For problems involving scattering or canonical field theories the relevant operators have continuous spectra. Systems with continuous variables can be approximated by discrete systems following section VII. In the continuous case a general Hamiltonian,  $H(p, x)$ , can be expressed as

$$H = \int \tilde{H}(p, x)U(x)V(p)dx dp \rightarrow \sum_{ij} \tilde{H}(p_j, x_i)U(x_i)V(p_j)dq_i dp_j \quad (103)$$

with a similar representation for the transfer matrix

$$T := e^{-iH\Delta t} = \int \tilde{T}(x, p)U(x)V(p)dx dp \rightarrow \sum_{ij} \tilde{T}(x_i, p_j)U(x_i)V(p_j)dx_i dp_j \quad (104)$$

where

$$\langle p|T|x\rangle = \tilde{T}(p, x)\langle p|x\rangle \quad \text{and} \quad \langle p|H|x\rangle = \tilde{H}(p, x)\langle p|x\rangle. \quad (105)$$

Here the quantities with the “tildes” are matrix elements of operators in a mixed basis where the canonical commutation relations are used to order the momentum operator to the left of the coordinate operators.

The probability amplitude can be expressed in terms of transfer matrices

$$\langle x_f|e^{-iHt}|x_i\rangle \quad (106)$$

is

$$\langle x_f|e^{-iHt}|x_i\rangle = \langle x_f|[e^{-iHt/N}]^N|x_i\rangle = \langle x_f|T^N|x_i\rangle. \quad (107)$$

Inserting intermediate states gives

$$\begin{aligned}
& \langle x_f | e^{-iHt} | x_i \rangle = \\
& \int \prod_i dp_i dx_i \langle x_f | p_N \rangle \langle p_N | T | x_N \rangle \langle x_N | p_{N-1} \rangle \langle p_{N-1} | T | x_{N-1} \rangle \cdots \\
& \quad \langle x_3 | p_2 \rangle \langle p_2 | T | x_2 \rangle \langle x_2 | p_1 \rangle \langle p_1 | T | x_1 \rangle \langle x_1 | x_i \rangle = \\
& \int \prod_i dp_i dx_i \langle x_f | p_N \rangle \langle p_N | x_N \rangle \tilde{T}(p_N, x_N) \langle x_N | p_{N-1} \rangle \times \\
& \quad \langle p_{N-1} | q_{N-1} \rangle \tilde{T}(p_{N-1}, x_{N-1}) \cdots \\
& \quad \langle x_3 | p_2 \rangle \langle p_2 | x_2 \rangle \tilde{T}(p_2, x_2) \langle x_2 | p_1 \rangle \langle p_1 | x_1 \rangle \tilde{T}(p_1, x_1) \langle x_1 | x_i \rangle. \tag{108}
\end{aligned}$$

This is exact; the Trotter limit justifies the replacement

$$\tilde{T}(p_i, x_i) \rightarrow e^{-i\tilde{H}(p_i, x_i)t/N} \tag{109}$$

as  $N \rightarrow \infty$ .

Completeness implies

$$\begin{aligned}
& P(x_f; p_N, x_N, \cdots, p_1, x_1) := \\
& \langle x_f | p_N \rangle \langle p_N | x_N \rangle \langle x_N | p_{N-1} \rangle \langle p_{N-1} | x_{N-1} \rangle \cdots \\
& \quad \langle x_3 | p_2 \rangle \langle p_2 | x_2 \rangle \langle x_2 | p_1 \rangle \langle p_1 | x_1 \rangle \tag{110}
\end{aligned}$$

satisfies

$$\int \prod_{i=1}^N dp_i dx_i P(x_f; p_N, x_N, \cdots, p_1, x_1) = 1 \tag{111}$$

independent of  $N$ . With the replacement (110) equation (108) becomes

$$\begin{aligned}
& \langle x_f | e^{-iHt} | x_i \rangle = \\
& \lim_{N \rightarrow \infty} \int \prod_i dp_i dx_i P(x_f; p_N, x_N, \cdots, p_1, x_1) \times \\
& \quad e^{-i \sum \tilde{H}(p_j, x_j)t/N} \delta(x_1 - x_i) \tag{112}
\end{aligned}$$

where the limit is interpreted as a strong limit; the initial coordinate must be multiplied by a wave packet and integrated. The complex probability interpretation follows by considering the integrals as Henstock integrals, which are limits of generalized Riemann sums. Cylinder



sets are defined by sets of paths that go through a generalized Riemann interval at each time step. The complex probability admits a factorization

$$\prod_{i=1}^N dp_i dx_i P(x_f; p_N, x_N, \dots, p_1, x_1) := \\ P(x_f; x_N, p_N) dx_N dp_N P(x_N; x_{N-1}, p_{N-1}) dx_{N-1} dp_{N-1} \dots \\ P(x_2; x_1, p_1) dx_1 dp_1 \quad (113)$$

which expresses the complex probability as a product of one step probabilities for each time step. Using this factorization gives

$$\langle x_f | e^{-iHt} | x_i \rangle = \\ \lim_{N \rightarrow \infty} \int \prod_i dp_i dx_i P(x_{i+1}; p_i, x_i) e^{-i\tilde{H}(p_i, x_i)t/N} \delta(x_1 - x_i), \\ x_{N+1} = x_f \quad (114)$$

In the discrete approximation of section VII the integrals are replaced by sums over the discrete values of  $p_m = m\epsilon$ ,  $x_m = m\epsilon$ ,  $dp_m = \epsilon = dp$  and  $dx_m = \epsilon = dx$  where  $-K \leq m \leq K$ ,  $M = 2K + 1$  and  $\epsilon^2 = \frac{2\pi}{M}$ . Equation (111) is still satisfied independent of the number  $M$  of discrete values of  $p_m$ ,  $x_m$ . In the discrete case a cylinder set is the set of paths that take on specific discrete values of  $p = n\epsilon$  and  $q = m\epsilon$  at each of the  $N$  intermediate time steps. In that case the complex probability for phase space paths becomes

$$P(x_f; p_N, x_N, \dots, p_1, x_1) \prod_i dp_i dx_i \rightarrow \\ P(x_f; p_{N i_N}, x_{N j_N}, \dots, p_{1 i_1}, x_{1 j_1}) \epsilon^{2N} := \\ \langle x_f | p_{N i_N} \rangle \epsilon \langle p_{N i_N} | x_{N j_N} \rangle \epsilon \langle x_{N j_N} | p_{N-1, i_{N-1}} \rangle \epsilon \langle p_{N-1, i_{N-1}} | x_{N-1, j_{N-1}} \rangle \epsilon \dots \\ \epsilon \langle x_{3 j_3} | p_{2 i_2} \rangle \epsilon \langle p_{2 i_2} | x_{2 j_2} \rangle \epsilon \langle x_{2 j_2} | p_{1 i_1} \rangle \epsilon \langle p_{1 i_1} | x_{1 j_1} \rangle \epsilon. \quad (115)$$

Here these indices represent the discrete momenta and coordinates that define a path in phase space. This has the property that the sum over all of the  $M^N$  cylinder sets for  $N$  intermediate time steps gives 1 independent of  $x_f$ . In this case there are cylinder sets of paths in both the  $p$  and  $x$  variables. These are considered as discrete approximations to the phase space paths,  $p(t)$ ,  $x(t)$ .

In the Trotter limit the discrete transfer matrix and discrete Hamiltonian (see (103)),

$$H = \sum \tilde{H}(p_m, x_n) U(x_n) V(p_m) \quad (116)$$

$$T = \sum \tilde{T}(p_m, x_n) U(x_n) V(p_m) \quad (117)$$

are related by

$$\tilde{T}(p_m, x_n) \approx e^{-i\tilde{H}(p_m, x_n)\Delta t}, \quad (118)$$

where this approximation preserves unitarity.

In this case

$$\begin{aligned} \langle x_f | e^{-iHt} | x_i \rangle = \\ \lim_{N \rightarrow \infty} \sum P(x_f; p_{N i_N}, x_{N j_N}, \dots, p_{1 i_1}, x_{1 j_1}) \times \\ e^{-i \sum \tilde{H}(p_{1 i_k}, x_{1 j_k}) t/N} \delta_{x_1, x_i} \end{aligned} \quad (119)$$

which expresses time evolution as the expectation of a complex probability on cylinder sets of paths in phase space. As in the continuous case the complex probability factors into a product of  $N$  one step complex probabilities:

$$\begin{aligned} P(x_f; p_{=N i_N}, x_{N j_N}, \dots, p_{1 i_1}, x_{1 j_1}) = \\ \prod_k [\langle x_{k+1 i_{k+1}} | p_{k i_k} \rangle \epsilon \langle p_{k i_k} | x_{k i_k} \rangle \epsilon] \quad x_{N+1} = x_f \end{aligned} \quad (120)$$

and the probability amplitude for a transition from  $x_i$  to  $x_f$  after time  $t$  becomes

$$\begin{aligned} \langle x_f | e^{-iHt} | x_i \rangle = \\ \lim_{N \rightarrow \infty} \sum \prod_k [\langle x_{k+1 i_{k+1}} | p_{k i_k} \rangle \epsilon \langle p_{k i_k} | x_{k i_k} \rangle \epsilon e^{-i\tilde{H}(p_{k i_k}, x_{k i_k}) t/N}] \delta_{x_1, x_i} \end{aligned} \quad (121)$$

where the sum is over cylinder sets. This reduces the calculation to computing powers of an  $M \times M$  matrix

When  $H$  has the form

$$H(p, x) = K(p) + V(x) \quad K(0) = 0 \quad (122)$$

equation (121) becomes

$$\begin{aligned} \langle x_f | e^{-iHt} | x_i \rangle = \\ \lim_{N \rightarrow \infty} \sum \prod_k [\langle x_{k+1 i_{k+1}} | p_{k i_k} \rangle \epsilon e^{-i\tilde{K}(p_{k i_k}) t/N} \langle p_{k i_k} | x_{k i_k} \rangle \times \end{aligned}$$

$$e^{-i\tilde{V}(x_{ki_k}t/N)\epsilon}]\delta_{q_1,q_i} \quad (123)$$

Since everything is finite the sums over the  $p$  values can be computed first, defining

$$P_X(x_f; x_{N i_N}, x_{N-1 i_{N-1}} \cdots x_{1 i_1}) := \sum_p \prod_k [\langle x_{k+1 i_{k+1}} | p_{k i_k} \rangle e^{-i\tilde{K}(p_{k i_k})t/N} \epsilon \langle p_{k i_k} | x_{k i_k} \rangle \epsilon] \quad (124)$$

which is complex valued function on cylinder sets of paths. It follows from (58), that summing over all of the cylinder sets, starting with the right most index and working to the left gives

$$\sum_x P_X(x_f; x_{N i_N}, x_{N-1 i_{N-1}} \cdots x_{1 i_1}) = e^{-iK(0)t} = 1. \quad (125)$$

With this definition

$$\langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \rightarrow \infty} \sum_q P_X(x_f, x_{N j_N}, \cdots, x_{1 j_1}) e^{-i \sum \tilde{V}(x_{1 j_k})t/N} \delta_{x_1, x_i}. \quad (126)$$

As in the general case the complex probability factors into products of conditional probabilities associated with each time step:

$$P_X(x_f; x_{N j_N}, \cdots, x_{1 j_1}) = \prod_k P_X(x_{k+1 i_{k+1}}; x_{k i_k}) \quad (127)$$

where

$$P_X(x_{k+1 i_{k+1}}; x_{k i_k}) = \sum_{p_{k i_k}} \langle x_{k+1 i_{k+1}} | p_{k i_k} \rangle e^{-i\tilde{K}(p_{k i_k})t/N} \epsilon \langle p_{k i_k} | x_{k i_k} \rangle \epsilon \quad (128)$$

which gives the following expression for the probability amplitude

$$\langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \rightarrow \infty} \sum \prod_k [P_X(x_{k+1 i_{k+1}}; x_{k i_k}) e^{-i\tilde{V}(x_{k i_k}t/N)}] \delta_{x_1 x_i} \quad (129)$$

This expresses the transition amplitude as the  $N^{\text{th}}$  power of a  $M \times M$  matrix.

Note that treating an infinite dimensional system as the limit of finite dimensional systems rather than discretizing the infinite dimensional system has some advantages. Discretizing was used in [7] where the rate of convergence was sensitive to how the points used to evaluate the interaction in each interval were chosen. The factorization of the complex probability

into products of conditional probabilities becomes approximate upon discretization. These choices could in principle affect unitarity numerically. These issues do not appear in the discrete case. In addition, the discrete analogs of the Fresnel integrals are well-defined finite sums. The complex probability interpretation arises naturally from the completeness relation.

## IX. SUMMARY AND CONCLUSION

This paper discusses an interpretation of the Feynman path integral for finite dimensional systems as the expectation value of a functional of paths with respect to a complex probability on cylinder sets of paths. This interpretation follows from the completeness relation and the Trotter product formula. While the passage from imaginary time to real time is problematical for an interpretation of the path integral as an integral, replacing the real-time integral by the expectation value of a functional on cylinder sets of paths with respect to a complex probability agrees with the Trotter limit. In the “phase space” form, based on Schwinger’s [10] discrete Weyl representation, it can be applied to any Hamiltonian matrix. Infinite dimensional systems can be approximated as limits of finite dimensional systems.

The complex probability approach provides an alternative way of thinking about path integrals. It is difficult to interpret the meaning of a discrete-valued function of a continuous time variable. One possible interpretation follows by noting that a sequence of discrete eigenvalues at different time steps are labels for transition amplitudes from the state at a given time step to another state at the next time step. All possible transition amplitudes are allowed at intermediate times between these successive time steps. In this sense a cylinder set of paths can be thought of as an ordered sequence of transition amplitudes between specific states at a sequence of time steps. The eigenvalues that label these amplitudes are the quantities normally associated with a classical path. The path integral is a complex weighted average over all ordered sequences of transition amplitudes. This provides a purely quantum mechanical interpretation of the path integral. This interpretation is natural when the complex probabilities are derived from the completeness relations.

The discrete representation has an equivalent qubit representation in terms of an irreducible set of elementary qubit gates. This representation may be more efficient for computational purposes since the complementary operators,  $U_i$  and  $V_i$  act on single qubits.

Discrete approximations to infinite dimensional systems are discussed in Appendix I and Appendix II. These applications demonstrate how this discrete formulation of the path integral can be applied to solve problems in potential scattering and quantum field theory. The path integral approach is not the most efficient way to perform scattering calculations, but the simple calculation presented in Appendix I, based time-dependent scattering theory, illustrates some of the issues need to be considered in future treatments of scattering formulated in terms of quantum computers.

In contrast to scattering problems, path integrals are one of the more direct methods to solve interacting field theories. The illustrated application to field theory in Appendix II uses a basis of wavelets to replace the fields by an infinite collection of almost local operators. Volume and resolution truncations are used to replace the field by a finite number of discrete modes. The calculations presented in Appendix II use a severe truncation of a  $\phi(x)^4$  field theory to two modes, but the calculation was completely non-perturbative. Realistic calculations are still a long way off.

## X. APPENDIX I: SCATTERING IN THE DISCRETE REPRESENTATION

Formal scattering theory is an idealization. A real scattering experiment takes place in a finite volume during a finite time interval. The relevant physics is dominated by a finite number of degrees of freedom that are limited by the energy and scattering volume.

The fundamental quantum mechanical observable is the probability for a transition from a prepared initial state to a detected final state

$$P_{fi} = |\langle \psi_f(t) | \psi_i(t) \rangle|^2. \quad (130)$$

While the individual states depend on time, the probability (130) is independent of  $t$  due to the unitarity of the time evolution operator. The important constraint is that both states have to be evaluated at the same time. The problem of scattering theory is that there is no common time when both the initial and final states are simple. On the other hand the initial state is simple before the collision and the final state is simple after the collision.

The initial and final states at the time of collision can be determined by evolving them from times where they behave like non-interacting subsystems to the collision time. Since localized wave packets spread, the effects of spreading can be eliminated by starting with

localized wave packets at the collision time, evolving them beyond the range of interactions using free time evolution, and then evolving them back to the interaction region using the full Hamiltonian. The result is a unitary mapping that transforms the free wave packet at the collision time to the dynamical wave packet at the same time.

If  $U_0(t)$  and  $U(t)$  represent the free and dynamical unitary time evolution operators, then assuming the time of collision is approximately at time  $t = 0$  the scattering asymptotic conditions have the form

$$\|U(\pm\tau)|\psi_{\pm}(0)\rangle - U_0(\pm\tau)|\psi_{0\pm}(0)\rangle\| \approx 0 \quad (131)$$

where the time  $\tau$  is sufficiently large for the interacting particles to be separated beyond the range of their mutual interactions. This expression is independent of  $\tau$  for sufficiently large  $\tau$ , but the minimum value of  $\tau$  depends on the range of the interaction and the structure of  $|\psi_{0\pm}(0)\rangle$ . Normally dependence on these conditions is removed by taking the limit  $\tau \rightarrow \infty$ . In this work, for computational reasons, it is desirable to choose  $\tau$  as small as possible, which requires paying attention to the range of the interaction and the structure of the initial and final states.

The unitarity of the time evolution operator means that (131) can be replaced by

$$\|\psi_{\pm}(0)\rangle - U(\mp\tau)U_0(\pm\tau)|\psi_{0\pm}(0)\rangle\| \approx 0 \quad (132)$$

for sufficiently large  $\tau$ . The operators

$$\Omega_{\pm}(\tau) := U(\pm\tau)U_0(\mp\tau) \quad (133)$$

are unitary mappings from  $|\psi_{0\pm}(0)\rangle$  to  $|\psi_{\pm}(0)\rangle$ .

Using these definitions the scattering probability can be expressed as

$$P_{fi} = |\langle\psi_{+}(0)|\psi_{-}(0)\rangle|^2 = |\langle\psi_{0+}(0)|S(\tau)|\psi_{0-}(0)\rangle|^2 \quad (134)$$

where

$$S(\tau) := \Omega^{\dagger}(\tau)\Omega(-\tau) \quad (135)$$

is the scattering operator. Since  $S(\tau)$  is unitary it can be expressed in terms of a self-adjoint phase shift operator

$$S(\tau) = e^{2i\delta(\tau)} \quad (136)$$

where  $S(\tau)$  should be independent of  $\tau$  for sufficiently large  $\tau$ .

In a real experimental measurement the probability (134) depends on the structure of the initial and final wave packets, which cannot be precisely controlled by experiment. If the matrix elements of  $S(\tau)$  in sharp-momentum states are slowly varying functions of momentum, then the dependence on the wave packet factors out [13] and can be eliminated to compute differential cross sections. In this case the sharp-momentum matrix elements can be approximated from the matrix elements using Gaussian (minimal uncertainty) wave packets with a “delta-function normalization” that are sharply peaked about the desired momenta.

This formulation of scattering admits a path integral treatment. As previously discussed scattering reactions are dominated by a finite number of degrees of freedom. The use of the discrete Weyl representation has the advantage that unitarity is exactly preserved on truncation to a finite number of degrees of freedom. Alternative path integral treatments of scattering appear in [14][15][16].

The advantage of the discrete representation is that  $U_0(-\tau)U(2\tau)U^0(-\tau)$  can be expressed as the limit of products of the transfer matrices defined section 8 (see (126)-(128))

$$S(\tau) = \lim_{N \rightarrow \infty} Y^{-N} X^{2N} Y^{-N} \quad (137)$$

where

$$Y_{ij} = P_X(x_i, x_j, \Delta t) \quad (X)_{ij} = P_X(x_i, x_j, \Delta t)e^{-iV(x_j)\Delta t}, \quad (138)$$

$\Delta t = \tau/N$  and  $N$  is the number of Trotter time slices. Note also that

$$Y^{-N} = P_X(x_f, x_i, -N\Delta t). \quad (139)$$

Sharp-momentum matrix elements of the scattering operator can be expressed in terms of the matrix elements of the transition operator,  $T$ , which is easier to calculate in the discrete representation

$$S = I - 2\pi i \delta(E_f - E_i) T \quad (140)$$

where  $T$  is approximately given by

$$T \approx V\Omega(-\tau) \quad (141)$$

when evaluated in normalizable states with sharply peaked momenta. The advantage of this representation is that for scattering problems  $V$  is a short range operator that provides a volume cutoff.

In the discrete representation sharp-momentum eigenstates are normalizable however *they cannot be used in scattering calculations* because they are completely delocalized in space since the discrete momenta and coordinates are complementary - making it impossible to get to the asymptotic region.

The most straightforward way to construct suitable initial or final wave packets in the discrete representation is to approximate the corresponding minimal uncertainty states of the continuum theory. The quantities to control are the mean position, momentum and the uncertainty in both of these quantities defined for a given state  $|\psi\rangle$  by:

$$\langle x \rangle_\psi := \sum_{n=-K}^K \frac{\langle \psi | u_n \rangle n \epsilon \langle u_n | \psi \rangle}{\langle \psi | \psi \rangle} \quad (142)$$

$$\langle p \rangle_\psi := \sum_{n=-K}^K \frac{\langle \psi | v_n \rangle n \epsilon \langle v_n | \psi \rangle}{\langle \psi | \psi \rangle} \quad (143)$$

$$\begin{aligned} (\Delta x)^2 &= \langle \psi | (x - \langle x \rangle)^2 | \psi \rangle = \\ &= \sum_{n=-K}^K \frac{\langle \psi | u_n \rangle ((n\epsilon)^2 - \langle x \rangle^2) \langle u_n | \psi \rangle}{\langle \psi | \psi \rangle} \end{aligned} \quad (144)$$

$$\begin{aligned} (\Delta p)^2 &= \langle \psi | (p - \langle p \rangle)^2 | \psi \rangle = \\ &= \sum_{n=-K}^K \frac{\langle \psi | v_n \rangle ((n\epsilon)^2 - \langle p \rangle^2) \langle v_n | \psi \rangle}{\langle \psi | \psi \rangle}. \end{aligned} \quad (145)$$

The continuum delta-function normalized minimal uncertainty states are

$$\langle p | \psi_0(0) \rangle = \frac{1}{2\sqrt{\pi}\Delta p} e^{-\frac{(p-\langle p \rangle)^2}{4(\Delta p)^2}}. \quad (146)$$

where  $\langle p \rangle$  is the mean momentum and  $\Delta p$  is the quantum mechanical uncertainty in  $p$  for this wave packet. This wave packet needs to be evolved to  $-\tau$  using the free time evolution which adds a phase to (146):

$$\langle p | \psi_0(-\tau) \rangle = \frac{1}{2\sqrt{\pi}\Delta p} e^{-\frac{(p-p_i)^2}{4(\Delta p)^2} + i\frac{p^2}{2\mu}\tau}. \quad (147)$$

In the discrete “ $p$ ” representation this is replaced by

$$\langle n | \psi_0(-\tau) \rangle = C e^{-\frac{(\epsilon n - \langle p \rangle)^2}{4(\Delta p)^2} + i\frac{n^2 \epsilon^2}{2\mu}\tau}. \quad (148)$$

where  $C$  is a normalization constant. In the  $x$  representation this becomes

$$\langle m | \psi_0(-\tau) \rangle = \frac{\epsilon}{\sqrt{2\pi}} \sum_{n=-K}^K e^{i\epsilon^2 mn} \langle n | \psi_0(-\tau) \rangle. \quad (149)$$



To illustrate that this gives a good approximation to the continuum results  $\langle p \rangle$ ,  $\langle x \rangle$ ,  $\Delta p$  and  $\Delta x$  were calculated starting with  $\langle p \rangle = 2.5$ ,  $\Delta p = .25$  and  $K = 300$  as input parameters in (147). The results of the calculation

$$\text{mean}_{p\text{-calc}} = 2.500000$$

$$\text{mean}_{x\text{-calc}} = 0.000000$$

$$\Delta_{p\text{-calc}} = .3000000$$

$$\Delta_{x\text{-calc}} = 1.666667$$

are consistent with the input parameters, the minimal uncertainty condition,  $\Delta p \Delta x = 1/2$  and the continuum results.

With these states the sharp-momentum half-shell transition matrix elements are

$$\langle p_f | T(E_i) | p_i \rangle \approx \langle \psi_{0f}(0) | V X^N | \psi_{0i}(-\tau) \rangle. \quad (150)$$

As a test the discrete approximation was applied to the problem of one-dimensional scattering of particle of mass  $m$  by a repulsive Gaussian potential of the form

$$V(q) = \lambda e^{-\alpha q^2} \quad (151)$$

with  $\lambda = .5$  and  $\alpha = 2.0$ . The potential is plotted in figure 1. The particle's mass is taken to be 1 in dimensionless units so the velocity and momentum can be identified. The initial wave packet is a Gaussian with a delta function normalization in momentum space with mean momentum  $p = 2.5$  and width  $\Delta p = .25$ . It is pictured in figure 2. The Fourier transform of the initial wave packet is given in figure 3. The oscillations are because the momentum space wave packet has a non-zero mean momentum. Given the size of the potential and wave packets, the wave packet needs to move about 18 units to the left in order to be out of the range of the potential. This suggest that for  $v = p/m = 2.5$  that  $\tau = 7$  should be sufficient to move the wave packet out of the range of the potential. The resulting free wave packet at  $\tau = -7$  is shown in figure 4. The scattered wave function with  $K = 300$  ( $M = 601$ ) after  $N = 100$  time steps is shown in figure 5, and that result multiplied by the potential is shown in figure 6. Compared to the wave function in figure 3, the wave function in figure 5 includes the effects of the interaction. Figure 6 illustrates the cutoff due to the short range potential; it shows how only the part of the wave function inside the range of the interaction contributes to the scattering operator. Figure 7 compares the result of the

off-shell Born approximation  $\langle p|V|\psi(0)\rangle$  to the calculation of the real and imaginary parts of  $\langle p|T|\psi(0)\rangle$  while figure 8 compares  $\langle p|T|\psi(0)\rangle$  to  $\langle p|T(p_0)|p_0\rangle$  obtained by numerically solving the Lippmann-Schwinger equation using the method [17].

Figure 8 shows that the path integral computation with an initial wave packet with a width of  $1/10$  of the momentum converges to the numerical solution of the integral equation. In unrelated time-dependent scattering calculations [18] a  $\Delta p$  of about a tenth of  $p$  gave good approximations to sharp momentum matrix elements of the transition operator for a wide range of momenta.

Unlike the solution of the Lippmann Schwinger equation, in the path integral approach for each energy it is necessary to determine minimal values of  $M, N, \tau$  and  $\Delta p$  that are needed for convergence. In practice there are a number of trade offs. Making the wave packets narrow in momentum increases the scattering volume in the coordinate representation. This in turn requires a larger  $\tau$  to get out of the range of the potential. If  $\tau$  gets too large the wave packet can move past  $q_{max} = K\epsilon$  and will reappear at  $q_{min} = -K\epsilon$ . As  $p$  gets large the oscillations in the  $q$  space wave function have higher frequencies, which requires smaller time steps, while when  $p$  gets small it is necessary to make the wave packet width in momentum small enough so the coordinate space tail of the wave function gets out of the interaction volume.

The computations require storing the initial vector. It is not necessary to store the one-step transfer matrix - it can be computed efficiently on the fly. This is important for realistic calculations since the vectors will be significantly larger in higher dimensions. The hope is that in the future qubits can be used to represent large vectors.

This one-dimensional example approximated half-shell sharp-momentum transition matrix elements. The on-shell values can be used to extract other observables such as phase shifts and in the one-dimensional case transmission and reflection coefficients. This formulation of the one-dimensional problem in terms of transition matrix elements has the advantage that the method can be formally be used in higher dimensions and to treat complex reactions or scattering in quantum field theory.

The formulation of the discrete path integral used the discrete Schwinger representation based on a single pair of complementary operators where the complex one time step probability is represented by a dense matrix. An equivalent representation in terms of qubits involves tensor products of matrices (74-75) that act on single qubits, which may have computational

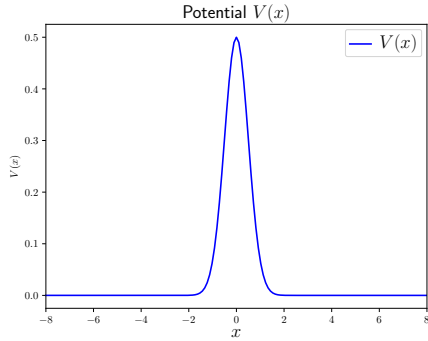


FIG. 1: **Potential**

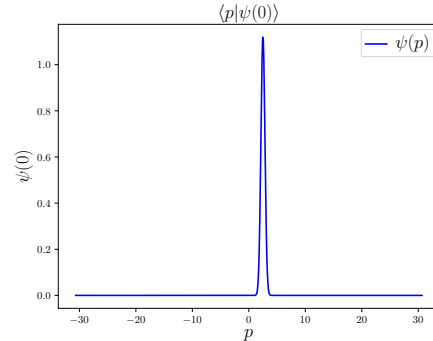


FIG. 2: **Momentum space initial Gaussian wave packet**

advantages.

One observation from these calculations that will have an impact on future computations using quantum computers is that width of the wave packets, total time for scattering, the scattering energy, the number of time steps and the resolution of the discretization all have to be considered together in order ensure an efficient calculation. This is because each one of these approximations generates its own source of errors that impact the errors in the other approximations.

The general strategy discussed above can also principle be utilized to formulate scattering quantum field theory. The Haag-Ruelle formulation of scattering [19][20][21][22] is the natural field-theoretic generalization of the quantum mechanical treatment of time dependent scattering. Like ordinary quantum mechanical scattering it uses strong limits and needs one-body (i.e. bound state) solutions to formulate the scattering asymptotic conditions.

## XI. APPENDIX: DISCRETE MULTI-RESOLUTION REPRESENTATION OF QUANTUM FIELD THEORY

One motivation for studying quantum computing in physics is that it might provide a framework for a numerical treatment of problems in strongly interacting quantum field theory. Clearly this goal is a long way off for realistic theories, but the state of quantum computing is advancing rapidly. Discrete formulations of field theory naturally fit into the discrete framework discussed in this work and should be relevant for future applications.

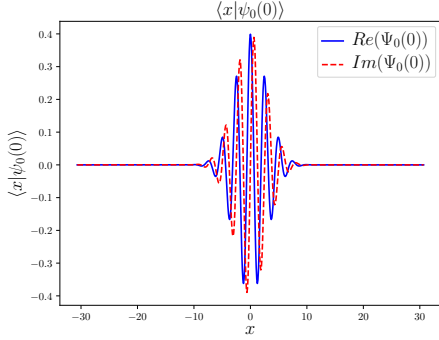


FIG. 3: Coordinate space initial Gaussian wave packet

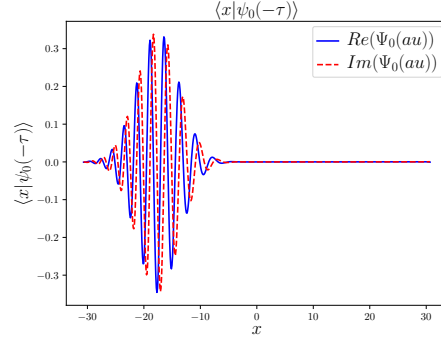


FIG. 4: Free Gaussian wave packet at  $\tau = -4$

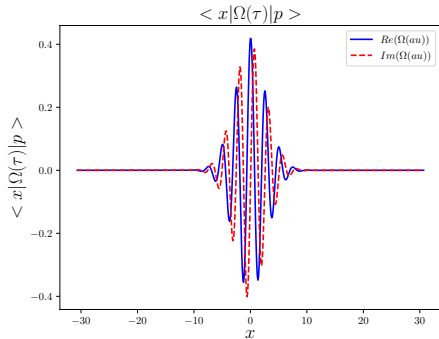


FIG. 5: Initial scattering state at  $t = 0$

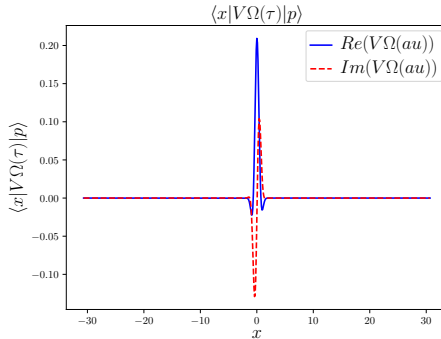


FIG. 6:  $\mathbf{V} \times$  initial scattering state at  $t = 0$

Discrete truncations to a small number of degrees of freedom can be used as a laboratory to explore how different field modes interact in a more realistic truncation of the theory.

A numerical treatment of quantum field theory requires a truncation to a system with a finite number of degrees of freedom. For reactions that take place in a finite space-time volume and involve a finite energy it is natural to limit the number of degrees of freedom by making volume and resolution truncations. Degrees of freedom that are outside of this volume or energetically inaccessible due to their resolution are expected to be unimportant for the given reaction. Daubechies wavelets [23][24][25] and scaling functions are a basis of square integrable functions and a natural representation to perform both kinds of truncations. The basis consists of a complete orthonormal set of functions that have compact support and a limited amount of smoothness. They have the property that in any small

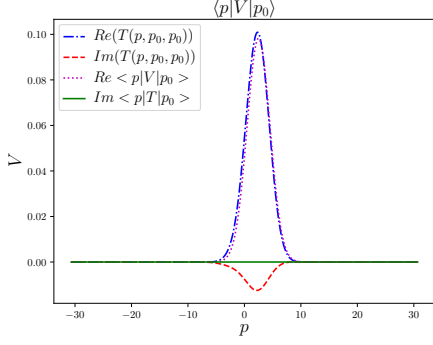


FIG. 7:  $\langle p|V|\psi_{0i}(0)\rangle$

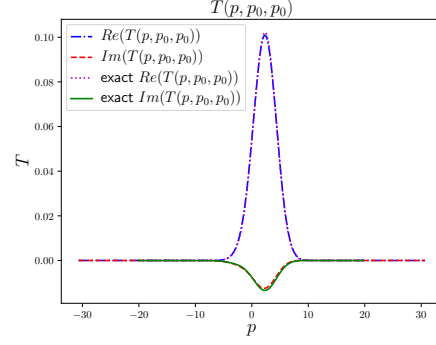


FIG. 8:  $\langle p|T|\psi_{0i}(0)\rangle$

volume there are an infinite number of basis functions supported entirely in that volume. This means that they can be used to construct “local” observables by smearing the fields with basis functions. All of the basis functions  $\xi_n(x)$  are generated from the solution of a linear renormalization group equation by translations and dyadic scale transformations, which facilitates computations. Because they are complete they can be used to *exactly* expand the canonical fields

$$\Phi(\mathbf{x}, t) = \sum \Phi_n(t) \xi_n(\mathbf{x})$$

$$\Pi(\mathbf{x}, t) = \sum \Pi_n(t) \xi_n(\mathbf{x})$$

where

$$\Phi_n(t) := \int d\mathbf{x} \Phi(\mathbf{x}, t) \xi_n(\mathbf{x})$$

and

$$\Pi_n(t) := \int d\mathbf{x} \Pi(\mathbf{x}, t) \xi_n(\mathbf{x})$$

are discrete field operators. If the fields satisfy canonical equal-time commutation relations

$$[\Phi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = i\delta(\mathbf{x} - \mathbf{y}) \quad (152)$$

then the discrete fields  $\Phi_n$  and  $\Pi_n$  will satisfy discrete versions of the canonical equal time commutation relations [26] [27] [28]:

$$[\Phi_m(t), \Pi_n(t)] = i\delta_{mn}$$

$$[\Phi_m(t), \Phi_n(t)] = 0$$

$$[\Pi_m(t), \Pi_n(t)] = 0. \quad (153)$$

In terms of these degrees of freedom the Hamiltonian for a  $\phi^4$  theory has the form

$$H = \frac{1}{2} \sum_n \Pi_n \Pi_n + \frac{m^2}{2} \sum_n \Phi_n \Phi_n + \sum_{mn} D_{mn} \Phi_m \Phi_n + \lambda \sum_{klmn} \Gamma_{klmn} \Phi_k \Phi_l \Phi_m \Phi_n \quad (154)$$

where the sum are all infinite. Since  $H$  commutes with itself the discrete fields in  $H$  can be evaluated at  $t = 0$ . The matrices in (154) are constants defined by the integrals

$$D_{mn} = \frac{1}{2} \int \nabla \xi_n(\mathbf{x}) \cdot \nabla \xi_m(\mathbf{x}) d\mathbf{x} \quad (155)$$

$$\Gamma_{klmn} = \int \xi_k(\mathbf{x}) \xi_l(\mathbf{x}) \xi_m(\mathbf{x}) \xi_n(\mathbf{x}) d\mathbf{x}. \quad (156)$$

For the wavelet basis these constants vanish unless all of the functions appearing in the integrals have a common support, which makes them almost local. In addition, because all of the functions in the integrand are related by translations and scale transformations to a single function, the integrals can all be expressed as linear combinations of solutions of some small linear systems generated by a renormalization group equation (see (157)). Unlike a lattice truncation, the wavelet representation of the field theory is (formally) exact (before truncation). The basis functions regularize the fields so local products of fields that appear in the Hamiltonian are replaced by infinite sums of well-defined products of discrete field operators. The basis functions are differentiable, so there are no finite difference approximations.

Wavelet representations of quantum field theories have been discussed by a number of authors [29] [30] [31] [32] [33] [34] [35] [36] [37] [38] [38] [39] [26] [40] [41] [42] [43] [44] [45] [46] [27] [47] [48] [28] [49] [50]. What is relevant is that the Hamiltonian (154) has the form  $\tilde{H} = \tilde{H}_1(p) + \tilde{H}_2(x) \rightarrow \tilde{H}_1(\Pi) + \tilde{H}_2(\Phi)$ , except it involves an infinite number of degrees of freedom. It is diagonal and quadratic in the discrete momentum operators and has a non-trivial (almost local) dependence on the  $\Phi_n$  operators.

The advantage of this basis is that it has natural volume and resolution truncations. For reactions taking place in a finite volume with a finite energy a finite number of these degrees of freedom should provide a good approximation. This reduces the problem to a problem with a finite number of discrete degrees of freedom. In addition the truncated Hamiltonian still has the form (154), except the sums are only over the retained discrete modes. As the

volume and resolution are increased (i.e as more modes are added) the parameters of the theory have to be adjusted to keep the some physical observables constant.

The truncated problem is a finite number of degree of freedom generalization of the one degree of freedom problem discussed in the section X.

The construction of the wavelet basis used to construct the discrete representation of the Hamiltonian (154) is outlined below. The starting point the solution of the linear renormalization group equation

$$s(x) = \sum_{l=0}^{2L-1} h_l DT^l s(x) \quad (157)$$

where

$$Df(x) := \sqrt{2}f(2x) \quad \text{and} \quad Tf(x) := f(x-1) \quad (158)$$

are unitary discrete dyadic scale transformations and unit translations. The  $h_l$  are constants that depend on the choice of  $L$ . Generally as  $L$  increases the solutions,  $s(x)$ , become smoother but the support increases. A useful case is  $L = 3$  where the solution  $s(x)$  of (157), called the scaling function, has support on  $[0, 2L-1] = [0, 5]$  and has one continuous derivative. In that case the coefficients  $h_l$  for the Daubechies  $L = 3$  scaling functions are

$$\begin{aligned} h_0 &= (1 + \sqrt{10} + \sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\ h_1 &= (5 + \sqrt{10} + 3\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\ h_2 &= (10 - 2\sqrt{10} + 2\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\ h_3 &= (10 - 2\sqrt{10} - 2\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\ h_4 &= (5 + \sqrt{10} - 3\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\ h_5 &= (1 + \sqrt{10} - \sqrt{5 + 2\sqrt{10}})/16\sqrt{2}. \end{aligned} \quad (159)$$

They are determined by the requirement that the solution of (157) and unit translates are orthonormal and locally finite linear combinations of these unit translates can be used to locally pointwise represent degree 2 polynomials. Given the solution,  $s(x)$ , of (157) new functions are constructed from  $s(x)$  by rescaling and translating

$$s_n^k(x) := D^k T^n s(x) = \sqrt{2^k} s(2^k x - n). \quad (160)$$

Since (157) is homogeneous in  $s(x)$  the starting scale can be fixed by requiring

$$\int s(x)dx = 1. \quad (161)$$

The functions  $s_n^k(x)$  for fixed  $k$  span a subspace of the square integrable functions on the real line with a resolution  $2^{-k}L$ :

$$\mathcal{S}^k := \left\{ f(x) \mid f(x) = \sum_{n=-\infty}^{\infty} c_n s_n^k(x) \quad \sum_{n=-\infty}^{\infty} |c_n|^2 < \infty \right\}. \quad (162)$$

The renormalization group equation (157) implies

$$\mathcal{S}^k \subset \mathcal{S}^{k+1}. \quad (163)$$

It follows that

$$\mathcal{S}^{k+1} = \mathcal{S}^k \oplus \mathcal{W}^k. \quad (164)$$

where  $\mathcal{W}^k$  is the orthogonal complement of  $\mathcal{S}^k$  in  $\mathcal{S}^{k+1}$ . An orthonormal basis for the subspace  $\mathcal{W}^k$  is the “wavelet functions”:

$$w_n^k(x) = D^k T^n w(x) \quad (165)$$

where

$$w(x) := \sum_{l=0}^{2L-1} (-)^l h_{2L-1-l} D T^l s(x) \quad (166)$$

is called the “mother wavelet”. This decomposition can be continued to generate a multi-resolution decomposition of  $L^2(\mathbb{R})$

$$L^2(\mathbb{R}) = \mathcal{S}^k \oplus_{l=0}^{\infty} \mathcal{W}^{k+l}. \quad (167)$$

This results in a multi-resolution orthonormal basis for  $L^2(\mathbb{R})$

$$\{\xi_n(x)\}_{n=-\infty}^{\infty} := \{s_n^k(x)\}_{n=-\infty}^{\infty} \cup \{w_n^m(x)\}_{n=-\infty, l=k}^{\infty}. \quad (168)$$

For the choice  $L = 3$  the basis functions  $s_n^k(x)$  and  $w_n^k(x)$  have compact support on  $[2^{-k}n, 2^{-k}(n+5)]$ . All of the basis functions have one continuous derivative so the coefficients (155) are defined. The functions  $s_n^k(x)$  are like splines in that linear combinations can be used to locally pointwise represent degree 2 polynomials while the functions  $w_n^l(x)$  are orthogonal to the same polynomials on their support. The Fourier transforms of the



basis functions are entire functions due to their compact support. Orthonormal three dimensional basis functions are products of one-dimensional basis functions. In spite of these nice properties, the basis functions are fractal valued (since they are related to fixed points of a renormalization group equation) and cannot be written down in closed form.

In order to use this representation the constant coefficients  $D_{mn}$  and  $\Gamma_{n_1 \dots n_k}$  that appear in the Hamiltonian (154) need to be computed. Using scale transformations (158) and the renormalization group equation (157) they can all be expressed in terms of the integrals

$$d_n = \int \frac{ds(x)}{dx} \frac{ds(x-n)}{dx} dx \quad -4 \leq n \leq 4 \quad (169)$$

$$\gamma_{m,n,k} = \int s(x)s(x-m)s(x-n)s(x-k)dx \quad -4 \leq m, n, k \leq 4. \quad (170)$$

These integrals for different values of  $m, n, k$  are related to each other by finite linear equations derived from the renormalization group equation (157) and the scale fixing condition (161). These linear systems can formally be solved in terms of the coefficients  $h_l$  (159). The coefficients  $d_n$  are rational numbers and can be found in the literature on wavelets [51]. To find the  $\gamma_{mnk}$  requires finding eigenvalues of a  $9^3 \times 9^3$  matrix. This eliminates the need to be able to evaluate fractal valued functions. Alternatively the integrals  $\gamma_{mnk}$  can be approximated by noting that the renormalization group equation (157) and the scale fixing condition (161) can be used to exactly calculate the basis functions and their derivatives at all dyadic rational points. Since the functions and their derivatives are continuous and the dyadic rationals are dense this can be used to estimate these quantities and integrals involving these quantities to any desired accuracy.

In order to illustrate a path integral treatment of this system consider a truncation of the theory in 1+1 dimensions where only 2 adjacent modes of the Hamiltonian (154) are retained. In this case the overlap coefficients that appear in the Hamiltonian are related to  $d_n$  and  $\gamma_{lmn}$  by

$$D_{mn} = d_{n-m} \quad \text{and} \quad \Gamma_{klmn} = \gamma_{l-k, m-k, n-k} \quad (171)$$

The coefficients that couple adjacent modes can be expressed in terms of the following

quantities

$$\begin{aligned}
\Gamma_{0000} &= 0.9528539 \\
\Gamma_{0001} &= 0.0670946 \\
\Gamma_{0011} &= 0.0890895 \\
\Gamma_{0111} &= -0.1424536 \\
D_{00} &= 295./56. \\
D_{01} &= -356./105. \\
D_{10} &= D_{01} \\
D_{11} &= D_{00}.
\end{aligned}$$

where the  $\Gamma$  coefficients were computed by numerical integration using the trapezoidal rule with the basis functions evaluated at 256 dyadic points on their support. Convergence was verified using 512 dyadic points.

The truncated Hamiltonian in this case is

$$\begin{aligned}
H = \frac{1}{2} \sum_{n=0}^1 \Pi_n \Pi_n + \frac{m^2}{2} \sum_{n=0}^1 \Phi_n \Phi_n + \sum_{m,n=0}^1 D_{mn} \Phi_m \Phi_n + \\
\lambda \sum_{k,l,m,n=0}^1 \Gamma_{klmn} \Phi_k \Phi_l \Phi_m \Phi_n
\end{aligned} \tag{172}$$

where  $\Gamma_{0000} = \Gamma_{1111}$ ,  $\Gamma_{0001} = \Gamma_{0010} = \Gamma_{0100} = \Gamma_{1000}$ , etc.. The path integral treatment of the field theory in the discrete representation is a multi-dimensional generalization of the treatment for one degree of freedom where each field mode represents an independent degree of freedom.

A general numerical treatment involves a truncation and renormalization followed by two approximations. The truncation discards all but a finite number,  $F$ , of discrete degrees of freedom.

$$H \rightarrow H_F. \tag{173}$$

Ideally physics at a given energy scale and in a given volume should be dominated by a finite number of accessible degrees of freedom. The remaining degrees of freedom that are not expected to impact calculations at that given scale and volume are discarded. The truncated theory is renormalized by adjusting the parameters of the theory so a set of

observables agree with experiment. This gives the parameters a dependence on the choice of retained degrees of freedom. This is a truncation rather than an approximation. It assumes that no additional parameters need to be introduced beyond what appears in the truncated Hamiltonian and that there is a limit as the volume becomes infinite and resolution becomes arbitrarily small. This is followed by two approximations. The first approximation is to approximate the unitary time evolution operator for the truncated theory using the Trotter product formula with  $N$  time slices:

$$U_F(t) = e^{-iH_F t} = \lim_{N \rightarrow \infty} (e^{-iH_F(\Pi)\Delta t} e^{-iH_F(\Phi)\Delta t})^N \quad (174)$$

where  $\Delta t = t/N$  and

$$H_F = H_F(\Pi) + H_F(\Phi) \quad (175)$$

with

$$H_F(\Pi) := \frac{1}{2} \sum_n \Pi_n \Pi_n \quad (176)$$

and

$$H_F(\Phi) := \frac{m^2}{2} \sum_n \Phi_n \Phi_n + \sum_{mn} D_{mn} \Phi_m \Phi_n + \lambda \sum_{klmn} \Gamma_{klmn} \Phi_k \Phi_l \Phi_m \Phi_n \quad (177)$$

which expresses  $H_F$  as the sum of a part with only the  $\Pi_n$  fields and another part with only the  $\Phi_n$  fields. Since the discrete canonical pairs of field operators  $\Phi_n$  and  $\Pi_n$  satisfy canonical commutation relations they have a continuous spectrum on the real line. This is because each one of these complementary operators generates translations in the other operator. The last step is to approximate the continuous spectrum of the discrete field operators  $\Phi_n$  and  $\Pi_n$  by a collection of  $M = 2K + 1$  closely spaced eigenvalues  $\phi_n, \pi_n = n\epsilon$  where  $-K \leq n \leq K$  and  $\epsilon^2 = 2\pi/M$ . This is exactly what was done in the scattering example, except in this case there are  $F$  degrees of freedom where  $F$  is the number of retained discrete field modes. Unlike the truncation, both of these steps are mathematical approximations.

Let  $\langle \phi | \chi \rangle = \chi(n_1\epsilon, \dots, n_F\epsilon)$  be a localized function of the amplitudes of the  $F$  discrete field modes that represent an initial free wave packet.

The goal is to use path integrals to calculate the time evolution of these coupled modes. This gives a non-perturbative treatment of the truncated problem.

For the field theory, before truncation, in the discrete representation the path integral involves integrals over an infinite number of modes. The normalization of the complex probability  $P_X$  is such that summing over all modes in the absence of interactions gives 1. This means that *the only modes that contribute non-trivially to the time evolution are the retained modes*. The discrete approximation results in a sample space with a finite number of discrete paths.

The Trotter approximation is

$$\begin{aligned} \langle n_1, n_2, \dots, n_F | U_F(t) | \chi(0) \rangle = \\ \lim_{N \rightarrow \infty} \langle n_1, n_2, \dots, n_F | (e^{-iH_F(\Pi)\Delta t} e^{-iH_F(\Phi)\Delta t})^N | \chi(0) \rangle. \end{aligned} \quad (178)$$

This can be evaluated by inserting complete sets of eigenstates of the complementary fields between each of the operators. The following abbreviations are used for sums over intermediate states:

$$\int d\phi = \epsilon^F \sum_{n_1=-K}^K \cdots \sum_{n_F=-K}^K, \quad (179)$$

for vectors representing a value of the eigenvalues of each of the  $F$  independent  $\phi$  fields,

$$\phi = (n_1\epsilon, \dots, n_F\epsilon) \quad -K \leq n_i \leq K, \quad (180)$$

for vectors representing the value of the eigenvalues of each of the  $F$  independent  $\pi$  fields

$$\pi = (n_1\epsilon, \dots, n_F\epsilon) \quad -K \leq n_i \leq K \quad (181)$$

and

$$\gamma = (\phi_0, \phi_1, \dots, \phi_N) \quad (182)$$

for a “path” that ends at  $\phi_0$  where  $\phi_j$  ( $j > 0$ ) represents values of each of the  $\phi_n$  fields at each of  $N$  time steps.

The following definitions are generalizations of the definitions in section VIII:

$$P_X(\phi', \phi, \Delta t) := \sum_{\mathbf{n}''} \langle \phi' | \pi'' \rangle e^{-i\pi'' \cdot \pi'' \Delta t} \epsilon^F \langle \pi | \phi \rangle \epsilon^F. \quad (183)$$

It follows from (59) that  $P_X(\phi', \phi, \Delta t)$  has the property

$$\sum_{\mathbf{n}} P_X(\phi', \phi, \Delta t) = 1 \quad (184)$$

and

$$\begin{aligned}
& P_X(\phi_f, \phi_N, \dots, \phi_1) := \\
& P_X(\phi_f, \phi_N, \Delta t) P_X(\phi_N, \phi_{N-1}, \Delta t) \dots \\
& P_X(\phi_3, \phi_2, \Delta t) P_X(\phi_2, \phi_1, \Delta t)
\end{aligned} \tag{185}$$

also satisfies

$$\sum_{\gamma \in \Gamma} P_X(\phi_f, \phi_N, \dots, \phi_1) = 1. \tag{186}$$

Equation (185) represents the complex probability of a given path, where at each time slice each of the  $F$   $\phi$ 's has one of the  $M$  allowed values between  $-K\epsilon$  and  $K\epsilon$ . Removing the last factor of  $\epsilon^F$  and only summing over  $\phi_N \dots \phi_2$  gives the evolution due to free propagation

$$\langle \phi_f | e^{-\frac{i}{2} \mathbf{\Pi} \cdot \mathbf{\Pi} t} | \phi_1 \rangle = \sum_{\mathbf{n}_n \dots \mathbf{n}_1} P_X(\phi_f, \phi_N, \dots, \phi_1) \epsilon^{-F}. \tag{187}$$

The full path integral including the effects of the interaction can be expressed as the expectation of the following potential functional of the path  $\gamma$

$$W[\gamma] := e^{i \sum_n H_F(\phi_n) \Delta t} \tag{188}$$

with respect to the complex probability distribution (186), where  $H_F(\phi_n)$  represents the value of the  $\phi$ -dependent part of the Hamiltonian evaluated at the value of the path  $\gamma$  at the  $n$ -th time slice.

This gives the path integral approximation

$$\begin{aligned}
& \langle n_{1f}, n_{2f}, \dots, n_{Ff} | U_F(t) | \chi(0) \rangle = \\
& \sum_{\gamma} P_X(\phi_f, \phi_N, \dots, \phi_1) W[\gamma] \chi(\phi_1)
\end{aligned} \tag{189}$$

which again represents the path integral for fields as the expectation value of a potential functional with respect to a complex probability distribution. As in the one degree of freedom case this can be exactly factored into a product of one-time step operators

$$\begin{aligned}
& P_X(\phi_f, \phi_N, \dots, \phi_1) W[\gamma] = \\
& X(\phi_f, \phi_N, \Delta t) e^{i H_F(\phi_N) \Delta t} X(\phi_N, \phi_{N-1}, \Delta t) e^{i H_F(\phi_{N-1}) \Delta t} \dots \\
& X(\phi_3, \phi_2, \Delta t) e^{i H_F(\phi_2) \Delta t} X(\phi_2, \phi_1, \Delta t) e^{i H_F(\phi_1) \Delta t}.
\end{aligned} \tag{190}$$

This can be used to represent time evolution as the product of large approximate transfer matrices.

Each stage the calculation uses finite mathematics. The use of the finite Weyl representation exactly preserves unitarity at each level of approximation. Both the  $\phi$  and  $\pi$  transfer matrices are unitary and can be expressed exactly in the truncated model. This means that the discrete Trotter approximation to time evolution is exactly unitary.

Figures nine and ten show calculations of the initial real and imaginary parts of the two field modes. In this case the initial modes are real and taken to be Gaussians of the form

$$\langle \phi_1, \phi_2 | \psi \rangle = N e^{-\sum_{i=0}^1 (\phi_i - \langle \phi_i \rangle)^2 / (4\delta\phi_i^2)} \quad (191)$$

Figures 11 and 12 show the real and imaginary parts of the time  $t = .5$  evolved amplitudes of the two discrete modes with  $M = 41$  field values using  $N = 20$  Trotter steps.

Figures 13 and 14 show plots of the real and imaginary parts of  $\phi_1$  when  $\phi_2 = 0$  at  $T = 0$  and  $T = .5$ .

In the initial calculations the initial mean displacement and uncertainty of each mode was taken to be .5. The initial state has no imaginary part but one develops due to the non-zero displacement of the initial state. This truncation is too crude to contain any real physics, however it illustrates the application of the discrete path integral to fields.

A more drastic truncation of the discretization of the continuum could be used to explore the dynamics of fields with a larger number of modes.

The wavelet representation for the Hamiltonian satisfies a functional renormalization group equation that could be used to reduce the number of amplitudes. This relates infinite volume truncated Hamiltonians at different resolutions using a canonical transformation along with mass, wave function, and coupling constant renormalizations:

$$H_k(\Pi, \Phi, \mu, \lambda) = 2^k H_0(2^{-k}\Pi, 2^k\Phi, 2^{-2k}\mu, 2^{-2k}\lambda).$$

Realistic calculations require a large number of field modes. Time-dependent scattering calculations of the type discussed in section 9 also require volumes sufficiently large for the scattered fragments to become stable particles. These calculations cannot be performed on a classical computer and will still be very challenging on a quantum computer.

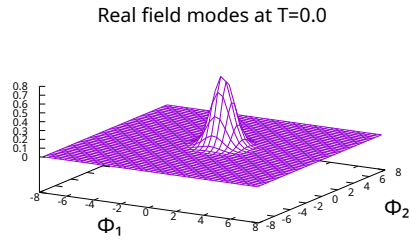


FIG. 9: Two modes (real) at  $T=0.0$

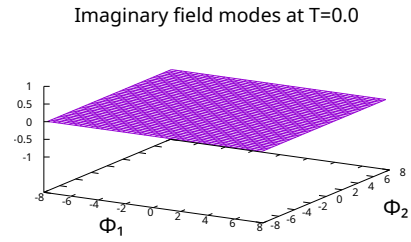


FIG. 10: Two modes (imaginary) at  $T=0.0$

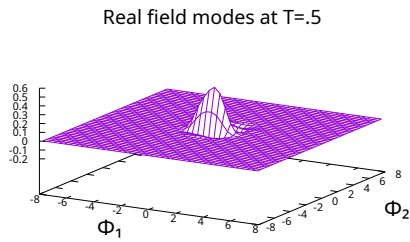


FIG. 11: Two modes (real) at  $T=0.5$

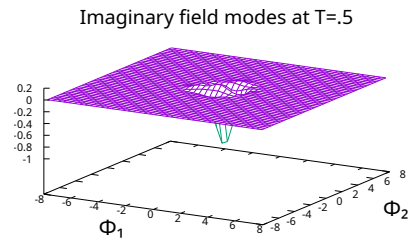


FIG. 12: Two modes (imaginary) at  $T=0.5$

---

[1] M. Reed and B Simon. *Methods of Modern Mathematical Physics*, volume I. Academic Press, San Diego, 1980.

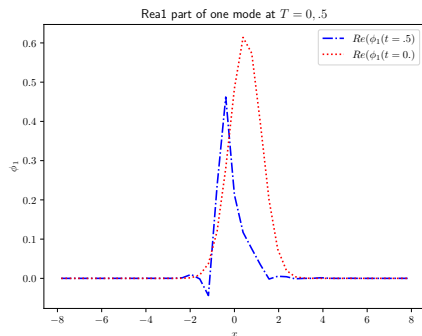


FIG. 13: One mode (real) at  $T=0.0$  and  $0.5$

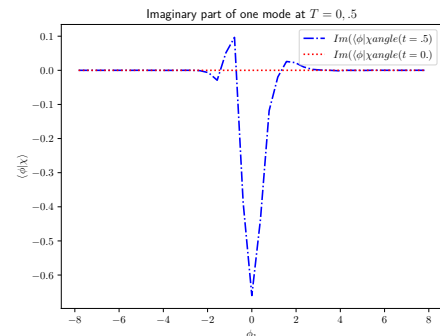


FIG. 14: One mode (imaginary) at  $T=0.0$  and  $0.5$

- [2] P. Muldowney. *A Modern Theory of Random Variation*. Wiley, N.J., 2012.
- [3] Ekaterina S. Nathanson and E.T. Jørgensen, Palle. A global solution to the Schrödinger equation: From Henstock to Feynman. *J. Math. Phys.*, 56:092102, 2015.
- [4] Ekaterina S. Nathanson. Path integration with non-positive distributions and applications to the Schrödinger equation. *University of Iowa Thesis*, 2015.
- [5] R. Henstock. *Theory of Integration*. Butterworths, London, 1963.
- [6] R. G. Bartle. *A Modern Theory of Integration, Graduate Studies in Mathematics*, volume 32. AMS, Providence, RI, 2000.
- [7] W. N. Polyzou and Ekaterina Nathanson. Scattering using real-time path integrals. *Phys. Rev. C*, 101:064001, Jun 2020.
- [8] P. Muldowney. Henstock on random variation. *Scientiae Mathematicae Japonicae Online*, e:657, 2007.
- [9] T. Gill and W. Zachary. Banach Spaces for the Feynman integral. *Real Analysis Exchange*, 34:1, 2008.
- [10] J. Schwinger and B-G. Englert ed. *Quantum Mechanics*. Springer, Berlin-Heidelberg, 2001.
- [11] Garrett Birkhoff and John Von Neumann. The Logic of Quantum Mechanics. *Annals of Mathematics*, 37(4):823–843, 1936.
- [12] H. Weyl. Quantenmechanik und gruppentheorie. *Zeitschrift für Physik*, 46:1, 1927.
- [13] W. Brenig and Haag R. General Quantum Theory of collision processes. *Fortsch. Phys.*, 7:183–242, 1959.
- [14] W. B. Campbell, P. Finkler, C. E. C. E. Jones, and M. N. Misheloff. Path-integral formulation of scattering theory. *Phys. Rev. D*, 12:2363, 1975.
- [15] R. Rosenfelder. Path integrals for potential scattering. *Phys. Rev. A*, 79:012701, 2009.
- [16] J. Carron and R. Rosenfelder. A new path-integral representation of the t-matrix in potential scattering. *Phys. Letters. A*, 375:3781, 2011.
- [17] O. A. Rubtsova, V. N. Pomerantsev, and V. I. Kukulin. Quantum scattering theory on the momentum lattice. *Physical Review C*, 79:064602, 2009.
- [18] P. Kopp and W. N. Polyzou. A Euclidean formulation of relativistic quantum mechanics. *Phys. Rev.*, D85:016004, 2012.
- [19] R. Haag. Quantum field theories with composite particles and asymptotic conditions. *Phys. Rev.*, 112:669–673, 1958.



- [20] W. Brenig and R. Haag. General quantum theory of collision processes. *Fort. der Physik*, 7:183, 1959.
- [21] D. Ruelle. On the asymptotic condition in quantum field theory. *Helv. Phys. Acta.*, 35:147, 1962.
- [22] R. Jost. *The General Theory of Quantized Fields*. AMS, 1965.
- [23] I. Daubechies. *Ten Lectures on Wavelets*, volume 61. SIAM, 1992.
- [24] O. Bratteli and P. E. T. Jørgensen. *Wavelets through a looking glass, The world of the spectrum*, volume 61. Birkhäuser, Boston, 2002.
- [25] P.E.T. Jørgensen. *Analysis and Probability, Wavelets, Signals, Fractals*, volume 234. Springer, NY, 2006.
- [26] Fatih Bulut and Wayne N. Polyzou. Wavelets in Field Theory. *Phys. Rev. D*, 87(11):116011, 2013.
- [27] W. N. Polyzou, Tracie Michlin, and Fatih Bulut. Multi-scale methods in quantum field theory. *Few Body Syst.*, 59(3):36, 2018.
- [28] W. N. Polyzou. Wavelet representation of light-front quantum field theory. *Phys. Rev. D*, 101(9):096004, 2020.
- [29] C. Best and A. Schaefer. Variational description of statistical field theories using Daubechies' wavelets. 1994.
- [30] P. Federbush. New formulation and regularization of gauged nonlinear wavelet expansion. *Prog. Theor. Phys.*, 94:1135, 1995.
- [31] I. G. Halliday and P. Suranyi. Simulation of field theories in wavelet representation. *Nuclear Physics B*, 436:414–427, February 1995.
- [32] G. Battle. *Wavelets and Renormalization, Series in Approximations and Decompositions, Volume 10*, volume 10. World Scientific, 1999.
- [33] C. Best. Wavelet induced renormalization group for the Landau-Ginzburg model. *Nucl. Phys. Proc. Suppl.*, 83:848, 2000.
- [34] A. E. Ismail, G. C. Rutledge, and G. Stephanopoulos. Multi-Resolution analysis in statistical mechanics. I. Using wavelets to calculate thermodynamic properties. *J. Chem. Phys.*, 118:4414, 2003.
- [35] A. E. Ismail, G. C. Rutledge, and G. Stephanopoulos. Multi-Resolution analysis in statistical mechanics. II. The wavelet transform as a basis for Monte Carlo simulations on lattices. *J.*

- Chem. Phys.*, 118:4424, 2003.
- [36] M. V. Altaisky. Wavelet-Based Quantum Field Theory Symmetry, Integrability and Geometry: Methods and Applications. *SIGMA*, 3:105, 2007.
- [37] S. Albeverio and M. V. Altaisky. A remark on gauge invariance in wavelet-based quantum field theory. 2009.
- [38] M. V. Altaisky. Quantum field theory without divergences. *Phys. Rev.*, D81:125003, 2010.
- [39] M. V. Altaisky and N. E. Kaputkina. Continuous Wavelet Transform in Quantum Field Theory. *Phys. Rev.*, D88:025015, 2013.
- [40] M. V. Altaisky and N. E. Kaputkina. On the wavelet decomposition in light cone variables. *Russ. Phys. J.*, 55:1177, 2013.
- [41] Gavin K. Brennen, Peter Rohde, Barry C. Sanders, and Sukhwinder Singh. Multiscale quantum simulation of quantum field theory using wavelets. *Phys. Rev. A*, 92:032315, Sep 2015.
- [42] Glen Evenbly and Steven R. White. Entanglement renormalization and wavelets. *Phys. Rev. Lett.*, 116:140403, Apr 2016.
- [43] M. V. Altaisky and N. E. Kaputkina. On quantization in light-cone variables compatible with wavelet transform. *Int. J. Theor. Phys.*, 55:2805, 2016.
- [44] M. V. Altaisky. Unifying renormalization group and the continuous wavelet transform. *Phys. Rev.*, D93:105043, 2016.
- [45] M. V. Altaisky. Wavelet view on renormalization group. 2016.
- [46] M. V. Altaisky. Wavelets and Renormalization Group in Quantum Field Theory Problems. *Physics of Atomic Nuclei*, 81:786, 2018.
- [47] H. Neuberger. Wavelets and lattice field theory. *EPJ Web of Conferences*, 175:11002, 2018.
- [48] E.T. Tomboulis. Wavelet field decomposition and UV opaqueness. *J. High Energy Physics*, 77, 2021.
- [49] Mikhail Altaisky, Natalia Kaputkina, and Robin Raj. Multiresolution quantum field theory in infinite-momentum frame. *Int. J. Theor. Phys.*, 61:46, 2022.
- [50] Mohsen Bagherimehrab, Yuval R. Sanders, Dominic W. Berry, Gavin K. Brennen, and Barry C. Sanders. Nearly optimal quantum algorithm for generating the ground state of a free quantum field theory. *PRX Quantum*, 3:020364, Jun 2022.
- [51] G. Beylkin. On the representation of operators in bases of compactly supported wavelets. *SIAM Journal on Numerical Analysis*, 29:1716, 1992.