Path integrals, complex probabilities and the discrete Weyl representation

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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 the 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.

Keywords: path integrals, quantum computing, complex probabilities

1. 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 of 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 $\Delta t \to 0$. 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 [2–4] 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 [2–4] 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 applications based on the complex probability interpretation of the path integral. While [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 are intuitive
and the Fresnel integrals are replaced by finite sums. Also in the finite dimensional case the complex probabilities exactly factor into products of conditional probabilities at each time step. Cylinder sets of paths are identified with ordered sequences of discrete eigenvalues of quantum observables at different intermediate times. Most of the ‘paths’ in a cylinder set are nowhere continuous. 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, as they would be in a quantum computer.

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 naturally formulated using a complex probability representation. In this work the dynamics is expressed as an average over a space of paths, the formal path integral is replaced by the expectation value of a functional of ‘classical paths’ with respect to a complex probability distribution on cylinder sets of paths. This reinterpretation of the path integral was developed in [2–4]. 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 [2, 5, 6], 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 section 2. The general treatment of discrete systems is discussed in section 3 and appendix A. 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 4 and appendix B. 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 cylinder sets 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 in section 5, the formulation of the discrete path integral in section 4 is expressed in terms of qubits in section 6. This is achieved by starting with an observable on a \(M = 2^L\) 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 a quantum system on an infinite dimensional Hilbert space as the limit of finite-dimensional systems discussed in section 7. The resulting formulation of the real-time ‘path integral’ is given in section 8. The application of the formalism to a simple model of a particle...
scattering off of a repulsive Gaussian potential is discussed in the section 9. The calculations utilize time-dependent methods which involve strong limits. Narrow wave packets in momentum are used to extract sharp-momentum transition matrix elements. In section 10 the application of these methods to local field theories is discussed. For field theories an additional discretization of the field amplitudes is needed for computations. In this section 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 the 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 construction of the wavelet basis is discussed in appendix C. The wavelet representation has natural volume and resolution trun-
cations. 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 discrete modes. While this is a drastic truncation, it illustrates how these discrete methods can used to model the dynamics of fields.

2. 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

$$P(S) = 1.$$  \hspace{1cm} (1)

$$P(S_i) + P(S_i^c) = 1$$  \hspace{1cm} (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 disjoint subsets of $S$

$$S_i \cap S_j = \emptyset, \quad i \neq j \quad P(\cup S_i) = \sum_i P(S_i).$$  \hspace{1cm} (3)

In the applications that follow the sample set, $S$, will be the set of cylinder sets of 'paths' that have discrete values at different times. A cylinder set is the collection of 'paths' that have 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 [2, 8].

In this work each cylinder set is associated with a collection of paths that have specific discrete values at each time step. By including additional time steps, the original set of paths is decomposed into subsets of paths with different values at the new intermediate times. Summing over the complex probabilities for these subsets of cylinder sets with different intermediate times gives the complex probability associated with the original cylinder set. This property demonstrates that the complex probability is defined consistently for any partition of the interval $[0,t]$ into a finite collection of time steps. The treatment of complex probabilities for continuously infinite dimensional path spaces is treated in [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].
3. Schwinger’s discrete Weyl algebra

This section summarizes Schwinger’s [10] method for 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. This section summarizes the main results of this construction. Details of Schwinger’s construction are presented in appendix A.

The construction starts with a quantum observable $X$ with $M$ orthonormal eigenvectors, $|m\rangle$, associated with $M$ possible measurement outcomes, $x_m$. $X$ is a $M \times M$ Hermitian matrix on a $M$-dimensional complex Hilbert space $H$. The outcomes are the eigenvalues of $X$:

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

The eigenvectors can be chosen to form an orthonormal basis on $H$. Schwinger defines a unitary operator $U$ on $H$ that cyclically shifts the eigenvectors of $X$:

$$U|m\rangle = |m+1\rangle \quad m < M \quad U|M\rangle = |1\rangle.$$  \hfill (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 $0 < k \leq M$, 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:

$$\lambda = u_m = e^{2\pi i m/M}$$  \hfill (6)

with orthonormal eigenvectors $|\bar{m}\rangle$:

$$U|\bar{m}\rangle = u_m|\bar{m}\rangle$$  \hfill (7)

$$\langle \bar{m}|\bar{n}\rangle = \delta_{mn}.$$  \hfill (8)

Next Schwinger defines a second unitary operator that cyclically shifts the eigenvectors of $U$ in the opposite direction

$$V|n\rangle = |n-1\rangle, \quad n \neq 1, \quad V|1\rangle = |M\rangle.$$  \hfill (9)

By definition

$$V^M = I$$  \hfill (10)

and

$$V|\bar{m}\rangle = v_m|\bar{m}\rangle \quad v_m = e^{2\pi i m/M}.$$  \hfill (11)

These definitions do not fix the phase of the eigenvectors of $U$ and $V$. The phases can be chosen so $|v_k\rangle = |k\rangle$ are the eigenvectors of the original observable, $X$. 


The operators $U$ and $V$ (see appendix A) have the following properties:

1. Any operator commuting with both $U$ and $V$ is a constant multiple of the identity.
2. $UV = VU e^{-i\pi/M}$
3. Any operator $O$ can be expressed as a degree $(M - 1) \times (M - 1)$ polynomial in $V$ and $U$
   \[
   O = \sum_{m,n=0}^{M-1} c_{mn} U^m V^n = \sum_{m,n=0}^{M-1} d_{mn} V^m U^n.
   \]

4. ‘Path integrals’ for finite dimensional systems

This section considers a general system of $M < \infty$ 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, $|\rangle_n$ for $1 \leq n \leq M$ is used to label these eigenvectors. $X$ will be called a ‘coordinate operator’ in this section, but in principle it can be any Hermitian operator on $H$.

The quantity of interest is the probability amplitude for a transition from an initial eigenstate $|\rangle_n$ of $X$ to a final eigenstate $|\rangle_m$ after time $t$. This is given by the matrix element,

\[
\langle n| e^{-iHt} |m\rangle,
\]

of the unitary time evolution operator. In this section (12) is expressed as the expectation value of a ‘functional of paths’ with respect to a complex probability on a space of paths [2–4].

Following the construction in section 3, irreducible pairs of unitary operators, $U$ and $V$, can be constructed from $X$. The eigenvectors $|\rangle_v_n$ of $V$ are identical to the eigenvectors, $|\rangle_n$, of $X$, while the eigenvectors $|\rangle_u_m$ of $U$ are complementary in the sense that

\[
\langle n| |\rangle_u_m\rangle = \frac{1}{M}
\]

for any $|\rangle_n$ and $|\rangle_m$. The operators $U$ and $V$ satisfy (A.4), (A.5), (A.14), (A.16) and

\[
VU = UV e^{i\pi/M}.
\]

The inner products of the eigenvectors of these complementary operators are

\[
\langle n| |\rangle_u_m\rangle = \frac{e^{-i2\pi mn/\sqrt{M}}}{\sqrt{M}}.
\]

The time-evolution operator can be expressed as the $N$th power of a unitary transfer matrix, $T$:

\[
e^{-iHt} = T^N \quad T = e^{-iH\Delta t} \quad \Delta t = t/N.
\]

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 (A.28):

\[
T = \sum_{mn} t_{mn} U^m V^n \quad H = \sum_{mn} h_{mn} U^m V^n.
\]
The quantities $t_{nm}$ and $h_{nm}$ are complex valued functions of two discrete variables. The eigenvalues of $X$ can be taken as one of the variables. For the purpose of comparing to path integrals expressed in terms of canonical coordinates and momenta it is useful to define another Hermitian operator, $P$, that has the same eigenvectors as $U$ with eigenvalues, $p_m$, analogous to the relation between $X$ and $P$,

$$ P|m\rangle = p_m|m\rangle. \quad (18) $$

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 in computations are the eigenvectors, $|m\rangle$. Matrix elements of the transfer matrix in a mixed basis of eigenvectors of $x$ and $p$ can be computed using (A.4), (A.5) and (A.16) in (17):

$$ \langle n|m\rangle \mathcal{T}_{nm} = \langle n|m\rangle \tilde{T}_{nm}, \quad (19) $$

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

$$ \tilde{T}_{nm} = \sum_{kl} t_{kl} e^{-\frac{2\pi i (m-n)}{N}}. \quad (20) $$

Mixed matrix elements of the Hamiltonian have a similar form

$$ \langle n|H|m\rangle = \langle n|m\rangle \tilde{H}_{nm} \quad \tilde{H}_{nm} = \sum_{kl} h_{kl} e^{-\frac{2\pi i (m-n)}{N}}. \quad (21) $$

Changing the ‘momentum’ $|m\rangle$ basis back to the ‘coordinate’ $|n\rangle$ basis gives

$$ \langle k|T|m\rangle = \sum_n \langle k|n\rangle \langle n|m\rangle \tilde{T}_{nm}. \quad (22) $$

and

$$ \langle k|H|m\rangle = \sum_n \langle k|n\rangle \langle n|m\rangle \tilde{H}_{nm}. \quad (23) $$

Matrix elements of the time evolution operator in the coordinate basis can be expressed, using representation (22) and (23) in (16), as

$$ \langle k|e^{-iHt/N}|k_i\rangle = \langle k| \left[ e^{-iHt/N} \right]^N |k_i\rangle = \sum_{k_1,\cdots,k_N} \langle k_j|T|k_N\rangle \langle k_N|T|k_{N-1}\rangle \cdots \langle k_2|T|k_1\rangle \langle k_1|T|k_i\rangle = \sum_{k_1,\cdots,k_N} \langle k_1|\tilde{n}_N\rangle \langle \tilde{n}_N|k_N\rangle \langle k_N|\tilde{n}_{N-1}\rangle \langle \tilde{n}_{N-1}|k_{N-1}\rangle \cdots \langle k_3|\tilde{n}_2\rangle \langle \tilde{n}_2|k_2\rangle \langle k_2|\tilde{n}_1\rangle \langle \tilde{n}_1|k_1\rangle \times \tilde{T}_{nk_1} \tilde{T}_{nk_2} \cdots \tilde{T}_{nk_N}. \quad (24) $$

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

If the $\tilde{T}_{nk}$ are all set to 1 then what remains after performing the completeness sums is the overlap of the final ‘coordinate’ with the initial ‘coordinate’, $\langle k|k_i\rangle = \delta_{k,k_i}$. 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:

$$P_N(k_f; n_N, k_N, \cdots n_1, k_1) := \langle k_f | \bar{n}_N \rangle \langle \bar{n}_N | k_N \rangle \langle k_N | \bar{n}_{N-1} \rangle \langle \bar{n}_{N-1} | k_{N-1} \rangle \times$$

$$\cdots \times \langle k_3 | \bar{n}_2 \rangle \langle \bar{n}_2 | k_2 \rangle \langle k_2 | \bar{n}_1 \rangle \langle \bar{n}_1 | k_1 \rangle$$

(25)

which by completeness satisfies

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

(26)

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.

Computation of the transfer matrix is equivalent to a diagonalization of the Hamiltonian, but for sufficiently small time steps it can be approximated without diagonalizing the Hamiltonian. This approximation becomes exact in the limit that the size of the time steps vanish, which is expressed using the Trotter product formula

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

(27)

where only the first-order term in time in the exponent contributes in the $N \to \infty$ limit. This limit converges strongly to $e^{-iHt}$ as $N \to \infty$ [1]. In the finite-dimensional case (27) follows from the identity $e^x = \lim_{N \to \infty} (1 + \frac{x}{N})^N$.

In the small $\Delta t = t/N$ limit

$$\langle \vec{m} | T[n] \rangle \approx \langle \vec{m} | I - iH\Delta t | n \rangle = \langle \vec{m} | n \rangle (1 - iH_{\text{int}} \Delta t) \approx \langle \vec{m} | n \rangle e^{-i\bar{H}_{\text{int}} \Delta t}.$$  

(28)

In this expression $H_{\text{int}}$ (21) is an ordinary function of $p_m$ and $x_n$.

If the quantum Hamiltonian $H$ is expressed with the $P$ operators to the right of the $X$ operators, $\bar{H}_{\text{int}}$ would be the Hamiltonian with these operators replaced by the ‘coordinates’ and ‘momenta’. It a discrete analog of a classical phase space Hamiltonian evaluated at a point in phase space.

It follows from (19) and (28) that

$$\bar{T}_{nk} \approx e^{-i\bar{H}(p_m, x_n) \Delta t}$$

and

$$\bar{T}_{n_k} \bar{T}_{n_{k-2}} \cdots \bar{T}_{n_2} \bar{T}_{n_1} \approx e^{-i \sum_{m=om} \bar{H}(p_m, x_m) \Delta t},$$

(29)

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, $p_m$ and $x_m$ at each time step. These ‘phase space’ paths are generally nowhere continuous. This is classical in the sense that even though the operators $P$ and $X$ do not commute, $\bar{H}(p_m, x_m)$ is an ordinary function of the eigenvalues $p_m$ and $x_m$. Following the definition in section 2 a cylinder set of paths is the set of all phase space paths, $p(t)$ and $x(t)$ that take on one of the $M$ possible eigenvalues of $P$ and $X$ at each of the $N$
time slices, subject to initial and final values of the ‘x’ variable. With this definition of cylinder set

\[ P_N(k_f; n_N, k_N, \cdots n_1, k_1) \]  

(30)
can be interpreted as a complex probability on the cylinder set of ‘phase space’ paths that start at \( x_{k_0} \), end at \( x_{k_f} \) and have values \( p_{n_m}, x_{n_m} \) at the \( m \)th time slice. This complex probability satisfies (1)–(3).

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

Combining (24), (25) and (28) for a sufficiently large \( N \) in the Trotter product formula gives the approximation

\[ \langle k_f \rangle e^{-iHt} |k_i \rangle \approx \sum_{n_0, k_N, \cdots n_1, k_1} P_N (k_f; n_N, k_N, \cdots n_1, k_1) e^{-i \sum_{m=0}^{N} \bar{H}(x_{n_m}p_{n_m}) \Delta t} \delta_{k_f, k_i} \]  

(31)

which converges in the limit that \( N \to \infty \). This approximates the transition probability amplitude as the expectation value of a functional of the ‘classical Hamiltonian’ \( \bar{H}(x, p) \) 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 (25) implies that the complex probability can be factored into a product of one-step probabilities

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

(32)

Using (32) the transition amplitude (12) can be approximated by

\[ \langle k_f \rangle e^{-iHt} |k_i \rangle \approx \prod_{n_0, k_N, \cdots n_1, k_1} \prod_{i} \left( P(k_{i+1}; n_i, k_i) e^{-i \bar{H}(x_{n_i}p_{n_i}) \Delta t} \right) \delta_{k_f, k_i} \]  

(33)

where \( k_{N+1} = k_f \). This reduces the computation of (31) to computing the \( N \)th power of a \( M \times M \) matrix.

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 for finite systems, since concept of continuously parameterized paths that have \( M \) possible values does not really make sense.

The advantage of this approach is that the time evolution is approximated by calculating the expectation value of a functional of a finite set of cylinder sets 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 paths in each cylinder set are generally nowhere continuous, the resulting amplitude is an entire function of time. While the limit for continuous time evolution exists [3, 4], real computations are truncated at a finite number of time steps.
The discrete path integral developed in section 4 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 non-commuting observables.

5. 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 statements have two possible outcomes; true or false. Different statements can be combined into compound statements which have two possible outcomes. The outcomes are determined by logical truth tables, which in turn can be represented by classical computer gates.

In a quantum system the presence of non-commuting observables complicates the logic. Specifically the results of measurements can depend on the order of the measurements. The propositional calculus behaves like properties of subspaces of a Hilbert space. States in quantum mechanics are identified with rays or one dimensional subspaces. Given another subspace in the Hilbert space there are three possibilities: the ray is in the subspace, the ray is orthogonal to the subspace, or the ray has a non-vanishing projection on the subspace and its orthogonal complement. Then the question ‘will the state always be measured to be in a particular invariant subspace of some operator $A$’ is always, never, or with a probability $P$ satisfying $0 < P < 1$. This feature can be represented using quantum gates associated with non-commuting operators, which can be modeled using irreducible sets of qubit gates. As an illustration consider a system in a spin up state in the $z$ direction. Measuring spin up in the $z$ direction will always give a positive result, measuring spin down in the $z$ direction will always give a negative result, but measuring spin up in the $x$ direction will give a positive result 50% of the time.

One consequence of the presence of non-commuting operators, pointed out by Birkhoff and Von Neuman [11], was that the distributive laws of classical logic

\[(A \land B) \lor C = (A \lor C) \land (B \lor C)\]
\[(A \lor B) \land C = (A \land C) \lor (B \land C)\]

can be violated in quantum systems when the statements $A$, $B$ and $C$ are associated with non-commuting operators.

6. 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 $M < K$. 

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

\[ n = \sum_{m=1}^{L} n_m 2^{m-1}. \tag{34} \]

This correspondence results in the identifications

\[ |u_{n_1 \cdots n_L}⟩ := |u_n⟩ \quad |v_{n_1 \cdots n_L}⟩ := |v_n⟩. \tag{35} \]

Define unitary operators $U_i$ and $V_i$ by

\[ U_i |v_{n_1 \cdots n_L}⟩ = |v_{n_1 \cdots [n_i+1] \mod 2 \cdots n_L}⟩ \tag{36} \]
\[ V_i |u_{n_1 \cdots n_L}⟩ = |u_{n_1 \cdots [n_i-1] \mod 2 \cdots n_L}⟩. \tag{37} \]

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

\[ U_i^2 - 1 = V_i^2 - 1 = 0, \tag{38} \]
\[ [U_i, U_j] = [V_i, V_j] = 0 \quad [U_i, V_j] = 0 \quad i \neq j. \tag{39} \]

Equation (A.23) for $M = 2$ gives

\[ V_i U_i = U_i V_i e^{i \pi}. \tag{40} \]

It follows from (34) that

\[ U^n = \prod_{m=1}^{L} U_{n_m}^m \tag{41} \]
\[ V^n = \prod_{m=1}^{L} V_{n_m}^m. \tag{42} \]

These equations can be understood by noting

\[ |v_n⟩ = U^n |v_0⟩ = U_1^{n_1} \cdots U_L^{n_L} |0, \ldots, 0⟩. \]

So each of the $2^L$ independent powers of $U$ (or $V$) can be expressed as a product of $U_i^0 = I$ or $U_i^1$ for $L$ different $U_i$ (or $V_i$). 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 given by the Pauli matrices $\sigma_1$ and $\sigma_3$:

\[ V_i = \sigma_3 \quad U_i = \sigma_1. \tag{43} \]

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

\[
\begin{align*}
|v_0\rangle &= \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & |v_1\rangle &= \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \\
|u_0\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, & |u_1\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.
\end{align*}
\]

The operators \( \sigma_1 \) and \( \sigma_3 \)

\[
U_i = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad V_i = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

satisfy (A.2) and (A.14) for \( M = 2 \):

\[
U_i |v_0\rangle|v_1\rangle, \quad U_i |v_1\rangle|v_0\rangle, \quad V_i |u_0\rangle|v_1\rangle, \quad V_i |u_1\rangle|v_0\rangle.
\]

They also satisfy

\[
\sigma_3 \sigma_1 = \sigma_1 \sigma_3 e^{i\pi/4}, \quad \left( \sigma_1^2 - 1 \right) = \left( \sigma_3^2 - 1 \right) = 0.
\]

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

\[
A = a_1 I + a_2 \sigma_1 + a_3 \sigma_3 + a_4 \sigma_3 \sigma_1.
\]

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 (41) and (42) relate the operators that appear in the discrete path integral to tensor products of single qubit operators \( \sigma_1 \) and \( \sigma_3 \). The irreducibility of the \( U_i, V_i \) operators implies that any gates involving several qubits can be expressed as products of these elementary gates. The advantage of these single qubit gates is that they are efficient at representing more complicated gates that involve a limited number of degrees of freedom.

7. 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

\[
\epsilon^2 := 2\pi / M.
\]

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 $M - 1 \leq n \leq M$. (For even $M$ the indices could be labeled $-M/2 + 1 \leq n \leq M/2$.) Discrete approximations to continuous variables $p$ and $x$ are defined by

$$p_l = le^{-i\frac{2\pi}{M}} \quad x_l = le^{-i\frac{2\pi}{M}} \quad -K \leq p_l, x_l \leq K$$  \hfill (50)

where

$$K = \sqrt{\frac{M\pi}{2}} - \sqrt{\frac{\pi}{2M}}.$$  \hfill (51)

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 $M \to \infty$ while at the same time the maximum and minimum values of $p_l$ and $x_l$, $p_{\pm K} = x_{\pm K} = \pm \epsilon = \epsilon$ approach $\pm \infty$ in the same limit.

While for finite $M$ any vector with a finite number of elements has a finite norm, in the continuum limit ($M \to \infty$) 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 $M \to \infty$ limit.

For unitary operators $U$ and $V$ given by (A.2) and (A.14) Hermitian operators $\hat{p}$ and $\hat{x}$ are defined by

$$V = e^{i\hat{p}} \quad U = e^{i\hat{x}}.$$  \hfill (52)

These can be used to define

$$V(x_m) = e^{i\hat{p}X m} = e^{i\hat{x}m} = V_m$$ \hfill (53)

$$U(p_n) = e^{i\hat{p}n} = e^{i\hat{x}n} = U^n.$$ \hfill (54)

With definitions (53) and (54) equation (A.23) becomes

$$V(x_m) U(p_k) = U(p_k) V(x_m) e^{i\epsilon x_k m} = U(p_k) V(x_m) e^{i\epsilon x m k} = U(p_k) V(x_m) e^{i\epsilon x m k}$$ \hfill (55)

which is the Weyl [12] (exponential) 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

$$dp = \epsilon dn = \sqrt{2\pi \frac{M}{M}} dn \quad dx = \epsilon dm = \sqrt{2\pi \frac{M}{M}} dm$$ \hfill (56)

and

$$\int dp \approx \sum_{n=-K}^{K} \frac{dp}{dn} = \epsilon \sum_{n=-K}^{K}$$ \hfill (57)

$$\int dx \approx \sum_{m=-K}^{K} \frac{dx}{dm} = \epsilon \sum_{m=-K}^{K}$$ \hfill (58)
which becomes a Riemann integral in the limit that \( M \to \infty \). It follows from (52) 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

\[
I = \sum_{l=-K}^{K} |v_l\rangle \langle v_l| = \sum_{l=-K}^{K} |p_l\rangle dp_l/p_l = \sum_{l=-K}^{K} |p_l\rangle \epsilon(p_l|)
\]

(59)

\[
I = \sum_{l=-K}^{K} |u_l\rangle \langle u_l| = \sum_{l=-K}^{K} |x_l\rangle dx_l/x_l = \sum_{l=-K}^{K} |x_l\rangle \epsilon(x_l|),
\]

(60)

which for finite \( \epsilon \) approximates the sum over small steps in \( p \) or \( x \) as integrals. Equations (59) and (60) imply the relations

\[
|p_l\rangle := |v_l\rangle / \sqrt{\epsilon}
\]

(61)

\[
|x_l\rangle := |u_l\rangle / \sqrt{\epsilon}.
\]

(62)

Using these identities gives

\[
\langle p_m| x_n \rangle = \frac{1}{\epsilon} \langle v_m| u_n \rangle = \frac{1}{\epsilon \sqrt{M}} e^{-i \frac{p_m x_n}{\epsilon}} = \frac{1}{\sqrt{2\pi}} e^{-i p_m x_n}
\]

(63)

\[
\langle p_m| p_n \rangle = \frac{1}{\epsilon} \langle v_m| v_n \rangle = \frac{\delta_{mn}}{\epsilon}
\]

(64)

and

\[
\langle x_m| x_n \rangle = \frac{1}{\epsilon} \langle u_m| u_n \rangle = \frac{\delta_{mn}}{\epsilon}
\]

(65)

In this notation equations (53) and (54) with (A.2) and (A.14) give

\[
U(x_m) |x_n\rangle = |x_m + x_n\rangle
\]

(66)

\[
V(p_m) |p_n\rangle = |p_m - p_n\rangle
\]

(67)

which can be expressed in terms of the ‘continuum variables’ as

\[
U(x) |x'\rangle = |x' + x\rangle
\]

(68)

\[
V(p) |p'\rangle = |p' - p\rangle.
\]

(69)

8. 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 7. In the continuous case a general Hamiltonian, \( H(p, x) \), can be approximated by

\[
H = \int \bar{H}(p, x) U(x) V(p) dx dp \approx \sum_{ij} \bar{H}(p_j, x_i) U(x_i) V(p_j) dx_i dp_j
\]

(70)
with a similar representation for the transfer matrix
\[
T := e^{-iH\Delta t} = \int T(x, p) U(x) V(p) \, dx \, dp \approx \sum_y \tilde{T}(x_i, p_j) U(x_i) V(p_j) \, dx_i \, dp_j
\] (71)

where
\[
\langle p|T|x \rangle = \tilde{T}(p, x) \langle p|x \rangle \quad \text{and} \quad \langle p|H|x \rangle = \tilde{H}(p, x) \langle p|x \rangle.
\] (72)

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 \( \langle x|e^{-iHt}|x_i \rangle \) can be expressed in terms of transfer matrices, \( T := e^{-iHt/N} \),
\[
\langle x|e^{-iHt}|x_i \rangle = \langle x \rangle \left( e^{-iHt/N} \right)^N \langle x_i \rangle = \langle x|T^N|x_i \rangle.
\] (73)

Inserting intermediate states gives
\[
\langle x|e^{-iHt}|x_i \rangle = \prod_i dp_i dx_i \langle x|p_N \rangle \langle p_N|T|N \rangle \langle N|p_N-1 \rangle \langle p_N-1|T|N-1 \rangle \cdots \langle x_3|p_2 \rangle \langle p_2|T|x_2 \rangle \langle x_2|p_1 \rangle \langle p_1|T|x_1 \rangle \langle x_1 \rangle 
\]
\[
= \prod_i dp_i dx_i \langle x|p_N \rangle \langle p_N|T|x_N \rangle \langle x_N|p_{N-1} \rangle \cdots \langle x_3|p_2 \rangle \langle p_2|T|x_2 \rangle \langle x_2|p_1 \rangle \langle p_1|T|x_1 \rangle \langle x_1 \rangle.
\] (74)

This is exactly \( \langle x \rangle \left( e^{-iH/N} \right)^N \langle x_i \rangle = \langle x|e^{-iHt/N}|x_i \rangle \). The Trotter limit justifies the replacement
\[
\tilde{T}(p_i, x_i) \rightarrow e^{-i\tilde{H}(p_i, x_i)/N}
\] (75)

which becomes exact in the limit \( N \rightarrow \infty \).

Completeness implies that
\[
P(x; p_N, x_N, \cdots, p_1, x_1) := \langle x|p_N \rangle \langle p_N|N \rangle \langle N|p_{N-1} \rangle \langle p_{N-1}|x_{N-1} \rangle \cdots \langle x_3|p_2 \rangle \langle p_2|x_2 \rangle \langle x_2|p_1 \rangle \langle p_1|x_1 \rangle.
\] (76)

Satisfies
\[
\int \prod_{i=1}^N dp_i dx_i P(x; p_N, x_N, \cdots, p_1, x_1) = 1
\] (77)

independent of \( N \). With the replacement (75) equation (74) becomes
\[
\langle x|e^{-iHt}|x_i \rangle = \lim_{N \rightarrow \infty} \int \prod_i dp_i dx_i P(x; p_N, x_N, \cdots, p_1, x_1)
\]
\[
\times e^{-i \sum \tilde{H}(p_i, x_i)/N} \delta(x_1 - x_i)
\] (78)
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

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

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

$$\langle x_f | e^{-iH(t)} | x_i \rangle = \lim_{N \to \infty} \int \prod_{i} dp_i dx_i P(x_{i+1}; p_i, x_i) e^{-i\tilde{H}(p, x) t/N} \delta(x_{i+1} - x_i),$$

$$x_{N+1} = x_f.$$  \hspace{1cm} (80)

In the discrete approximation of section 7 the integrals are replaced by sums over the discrete values of $p_m = \epsilon = dp$ and $x_m = \epsilon = dx$ where $-K \leq m \leq K$, $M = 2K + 1$ and $\epsilon^2 = \frac{\delta t}{M}$. Equation (77) 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 $p$ and $x$ at each of the $N$ intermediate time steps. In that case the complex probability for phase space paths becomes

$$P(x_f; p_N, x_N, \cdots, p_1, x_1) \prod_{i} dp_i dx_i \rightarrow P(x_f; p_{N_i}, x_{N_i}, \cdots, p_{1_i}, x_{1_i}) \epsilon^{2N}$$

$$\hspace{2cm} := \langle x_f | p_{N_i} \rangle \epsilon \langle x_{N_i} | x_{N_i} \rangle \epsilon \langle x_{N_i} | p_{N_i-1} \rangle \epsilon \langle p_{N_i-1} | x_{N_i-1} \rangle \epsilon \cdots \epsilon \langle x_{1_i} | p_{2_i} \rangle \epsilon \langle p_{2_i} | x_{2_i} \rangle \epsilon \langle x_{2_i} | p_{1_i} \rangle \epsilon \langle p_{1_i} | x_{1_i} \rangle \epsilon.$$  \hspace{1cm} (81)

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 (70)),

$$H = \sum \tilde{H}(p_m, x_m) U(x_m) V(p_m)$$

$$T = \sum \tilde{T}(p_m, x_m) U(x_m) V(p_m)$$

are related by

$$\tilde{T}(p_m, x_m) \approx e^{-i\tilde{H}(p_m, x_m) \Delta t},$$  \hspace{1cm} (84)

where this approximation preserves unitarity.
In this case
\[ \langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \sum_{N^q} \langle x_f \rangle P(x_f; p_{N|x_i}, x_{N|f}, \cdots, p_{N|1}, x_{N|1}) e^{-i \sum \tilde{H}(p_{k|x_i})/N} \delta_{x_i, x} \] (85)
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:
\[ P(x_f; p_{N|x_i}, x_{N|f}, \cdots, p_{N|1}, x_{N|1}) = \prod_k \left[ \langle x_{k+1|x_i} | p_{k|x_i} \rangle \langle p_{k|x_i} | x_{k|x_i} \rangle e^{-i\tilde{H}(p_{k|x_i})/N} \right] \delta_{x_i, x} \] (86)
and the probability amplitude for a transition from \( x_i \) to \( x_f \) after time \( t \) becomes
\[ \langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \sum_k \prod_p \left[ \langle x_{k+1|x_i} | p_{k|x_i} \rangle \langle p_{k|x_i} | x_{k|x_i} \rangle e^{-i\tilde{H}(p_{k|x_i})/N} \right] \delta_{x_i, x} \] (87)
where the sum is over cylinder sets. This reduces the calculation to computing powers of a \( M \times M \) matrix.

For the examples discussed in sections 9 and 10 \( H \) has the form
\[ H(p, x) = H_1(p) + H_2(x) \quad H_1(0) = 0 \] (88)
with
\[ \tilde{H}(p, x) = \tilde{H}_1(p) + \tilde{H}_2(x) \quad \tilde{H}_1(0) = 0. \]
This is discussed in detail in (appendix B). In this case equation (87) becomes
\[ \langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \sum_k \prod_p \left[ \langle x_{k+1|x_i} | p_{k|x_i} \rangle \langle p_{k|x_i} | x_{k|x_i} \rangle e^{-i\tilde{H}(p_{k|x_i})/N} \delta_{x_i, x} \right] \] (89)
Since everything is finite the sums over the \( p \) values can be computed first, defining
\[ P_X(x_f; x_{N|x_i}, x_{N-1|x_i}, \cdots, x_{N|1}) := \sum_p \prod_k \left[ \langle x_{k+1|x_i} | p_{k|x_i} \rangle \langle p_{k|x_i} | x_{k|x_i} \rangle e^{-i\tilde{H}(p_{k|x_i})/N} \right] \] (90)
which is complex valued function on cylinder sets of paths in the ‘\( x \)’ variable. It follows from (B.3), that summing over all of the cylinder sets, starting with the right most index and working to the left gives
\[ \sum x \langle x_f; x_{N|x_i}, x_{N-1|x_i}, \cdots, x_{N|1} \rangle = e^{-i\tilde{H}_1(0)t} = 1. \] (91)
With this definition
\[ \langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \sum_X P_X(x_f; x_{N|x_i}, \cdots, x_{N|1}) e^{-i \sum \tilde{H}_1(x_i)/N} \delta_{x_i, x}. \] (92)
As in the general case the complex probability factors into products of conditional probabilities associated with each time step:

$$P_X(x_f; x_{Nj}, \ldots, x_{1j}) = \prod_k P_X(x_{k+1}; x_{ki})$$  \hspace{1cm} (93)

where

$$P_X(x_{k+1}; x_{ki}) = \sum_{p_{ki}} \langle x_{k+1} | p_{ki} \rangle e^{-i\tilde{H}_1(x_{ki})t/N} \delta(x_{ki})$$  \hspace{1cm} (94)

which gives the following expression for the probability amplitude

$$\langle x_f | e^{-iHt} | x_i \rangle = \lim_{N \to \infty} \sum_k \prod_k \left[ P_X(x_{k+1}; x_{ki}) e^{-i\tilde{H}_2(x_{ki})t/N} \right] \delta_{t, t_i}.$$  \hspace{1cm} (95)

This expresses the transition amplitude as the $N$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.

9. 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

$$P_{fi} = |\langle \psi_f(t) | \psi_i(t) \rangle|^2.$$  \hspace{1cm} (96)

While the individual states depend on time, the probability (96) 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.

For scattering the Hamiltonian $H$ is the sum of a free Hamiltonian $H_0$ and an interaction $V$. In this section $U(t)$, $V$, $T(z)$ represent the unitary time translation operator, the potential, and the transition operator rather than the Weyl operators and the transfer matrix.
If \( U_0(t) \) and \( U(t) \) represent the free and dynamical unitary time evolution operators, \( e^{-iH_0 t} \) and \( e^{-iHt} \), then assuming the time of collision is approximately at time \( t = 0 \) the scattering asymptotic conditions have the form

\[
\| U(\pm \tau) |\psi_{\pm}(0)\rangle - U_0(\pm \tau) |\psi_{0\pm}(0)\rangle \| \approx 0
\]

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, \( V \), and the structure of \( |\psi_{0\pm}(0)\rangle \). Normally the dependence on these conditions is removed by taking the limit \( \tau \to \infty \).

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 (97) can be replaced by

\[
\| |\psi_{\pm}(0)\rangle - U(\mp \tau) U_0(\pm \tau) |\psi_{0\pm}(0)\rangle \| \approx 0
\]

for sufficiently large \( \tau \). The operators

\[
\Omega_{\pm}(\tau) := U(\pm \tau) U_0(\mp \tau)
\]

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

Using these definitions the scattering probability can be expressed as

\[
P_f = |\langle \psi_{\pm}(0) |\psi_{-}(0)\rangle|^2 = |\langle \psi_{0\pm}(0) |S(\tau) |\psi_{0-}(0)\rangle|^2
\]

where

\[
S(\tau) := \Omega(\tau)\Omega(-\tau)
\]

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

\[
S(\tau) = e^{2i\delta(\tau)}
\]

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

In a real experimental measurement the probability (100) 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 [14–16].

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 in section 7 (see (92) and (95))

\[
S(\tau) = \lim_{N \to \infty} Y^{-N}X^{2N}Y^{-N}
\]
where
\[ Y_{ij} = P_X(x_i, x_j, \Delta t) \]
\[ (X)_{ij} = P_X(x_i, x_j, \Delta t) e^{-iV(x_j)\Delta t}, \]
(104)

\[ \Delta t = \tau/N \] and \( N \) is the number of Trotter time slices. Note also that
\[ Y^{N} = P_X(x_f, x_i, -N\Delta t). \]
(105)

Sharp-momentum matrix elements of the scattering operator can be expressed in terms of the matrix elements of the transition operator,
\[ T(z) = V + V(z - H)^{-1} V \]

\[ \langle p_f|S|p_i \rangle = \langle p_f|p_i \rangle - 2\pi i \delta(E_f - E_i) \langle p_f|T(E + i\epsilon)|p_i \rangle \]
(106)

where \( T \) is approximately given by [13]
\[ T(E + i\epsilon) \approx V\Omega(-\tau) \]
(107)

when evaluated in normalizable states with sharply peaked momenta. This becomes exact in the limit \( \tau \to \infty \). The advantage of this representation is that for scattering problems the interaction \( V \) is a short range operator that provides a volume cutoff.

In the discrete representation sharp-momentum eigenstates are normalizable however \textit{they cannot be used in scattering calculations} because they are completely delocalized in space, since the discrete momenta and coordinates are complementary operators - 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:
\[ \langle x \rangle_\psi := \sum_{n=-K}^{K} \frac{\langle p|u_n\rangle n e^{-\langle x \rangle_\psi^2}}{\langle p|p \rangle} \]
(108)

\[ \langle p \rangle_\psi := \sum_{n=-K}^{K} \frac{\langle p|v_n\rangle n e^{-\langle p \rangle_\psi^2}}{\langle p|p \rangle} \]
(109)

\[ (\Delta x)^2 = \langle x \rangle (x - \langle x \rangle)^2 |\psi \rangle = \sum_{n=-K}^{K} \frac{\langle p|u_n\rangle \left( (ne)^2 - \langle x \rangle^2 \right) \langle u_n|\psi \rangle}{\langle p|p \rangle} \]
(110)

\[ (\Delta p)^2 = \langle p \rangle (p - \langle p \rangle)^2 |\psi \rangle = \sum_{n=-K}^{K} \frac{\langle p|v_n\rangle \left( (pe)^2 - \langle p \rangle^2 \right) \langle v_n|\psi \rangle}{\langle p|p \rangle}. \]
(111)

The continuum delta-function normalized minimal uncertainty states are
\[ \langle p|\psi_0(0) \rangle = \frac{1}{2\sqrt{\pi} \Delta p} e^{-\frac{(p - \langle p \rangle)^2}{4\Delta p^2}}. \]
(112)
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 (112):

\[
\langle p | \psi_0 (-\tau) \rangle = \frac{1}{2\sqrt{\pi} \Delta p} e^{-\frac{(p - \langle p \rangle)^2}{4\Delta p^2}} e^{\frac{i}{\hbar} p^2 \tau}. \tag{113}
\]

In the discrete ‘\( p \)’ representation this is replaced by

\[
\langle n | \psi_0 (-\tau) \rangle = C e^{-\frac{(\epsilon_n - \langle p \rangle)^2}{4\Delta p^2}} e^{\frac{i}{\hbar} \epsilon_n^2 \tau}. \tag{114}
\]

where \( C \) is a normalization constant. In the \( x \) representation this becomes

\[
\langle m | \psi_0 (-\tau) \rangle = \frac{\epsilon}{\sqrt{2\pi}} \sum_{n=-K}^{K} e^{i\epsilon mn} \langle n | \psi_0 (0) \rangle. \tag{115}
\]

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 (113). The results of the calculation

- mean\(_p\)-calc = 2.500000
- mean\(_x\)-calc = 0.000000
- \( \Delta p \)-calc = .3000000
- \( \Delta x \)-calc = 1.666667

are consistent with the input parameters, the minimal uncertainty condition, \( \Delta p \Delta x = \frac{1}{2} \), and the continuum results.

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

\[
\langle p | T(E_i) | p_i \rangle \approx \langle \psi_0 (0) | VX^N | \psi_0 (-\tau) \rangle. \tag{116}
\]

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

\[
V(x) = \lambda e^{-\alpha x^2} \tag{117}
\]

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 can be identified with the momentum. 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 tradeoffs. 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 \( x_{\text{max}} = K\epsilon \) and will reappear at \( x_{\text{min}} = -K\epsilon \). As \( p \) gets large the oscillations in
Figure 3. Coordinate space initial Gaussian wave packet.

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

Figure 5. Initial scattering state at $t = 0$. 
Figure 6. $V \times$ initial scattering state at $t = 0$.

Figure 7. $\langle p|V|\psi(0)\rangle$.

Figure 8. $\langle p|T|\psi(0)\rangle$.
the $x$ 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 (41) and (42) that act on single qubits, which may have computational 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 for an accurate and 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 [13, 19–21] 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.

10. 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. 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 [22–24] 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 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. The construction of the basis is discussed in (appendix C). Because they are complete they can be used to exactly expand the canonical fields

$$\Phi(x,t) = \sum \Phi_n(t) \xi_n(x) \quad \Pi(x,t) = \sum \Pi_n(t) \xi_n(x)$$

where

$$\Phi_n(t) := \int dx \Phi(x,t) \xi_n(x) \quad \Pi_n(t) := \int dx \Pi(x,t) \xi_n(x)$$

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

$$[\Phi(x,t), \Pi(y,t)] = i \delta(x-y)$$

then the discrete fields $\Phi_n$ and $\Pi_n$ will satisfy discrete versions of the canonical equal time commutation relations \[25–27\]:

$$[\Phi_m(t), \Pi_n(t)] = i \delta_{mn}$$
$$[\Phi_m(t), \Phi_n(t)] = 0$$
$$[\Pi_m(t), \Pi_n(t)] = 0.$$

In terms of these degrees of freedom the Hamiltonian for a $\phi^4$ theory has the form \[25, 26\]

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

where the sum are all infinite. Since $H$ commutes with itself the discrete fields in $H$ can be evaluated at $t = 0$.

The equal time canonical commutation relations (119) imply that the momentum modes generate translations of the field modes and the field modes generate translations of the momentum modes. This means that the spectrum of both $\Phi_n$ and $\Pi_n$ is the real line. In the discrete approximation the amplitude of each field mode is replaced by a large finite set of points that approach the continuum following the construction in section 7. The cylinder sets of paths for each mode are ‘paths’ that take on the value of one of these points at each time slice. The total cylinder set is the product of these sets over all retained $\Phi_n$ and $\Pi_n$ modes. This means that if $M$ $\Phi_n$ and $\Pi_n$ modes are retained, there are $2^M$ sequences of discrete values representing $2^M$ cylinder sets of paths. In a truncation the discarded modes do not contribute to the dynamics since their complex probabilities sum to 1, so it is only necessary to determine the dynamics of the retained modes.

The matrices in (120) are constants defined by the integrals

$$D_{mn} = \frac{1}{2} \int \nabla \xi_n(x) \cdot \nabla \xi_m(x) dx$$
$$\Gamma_{klmn} = \int \xi_k(x) \xi_l(x) \xi_m(x) \xi_n(x) dx$$
where
\[ \nabla = \hat{x} \frac{\partial}{\partial x} + \hat{y} \frac{\partial}{\partial y} + \hat{z} \frac{\partial}{\partial z} \]
is the gradient operator. 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 to a single function by translations and scale transformations, the integrals can all be expressed as linear combinations of solutions of some small linear systems of equations generated by the renormalization group equation (see (C.1)) \[25, 27\]. 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 [25–37, 37–49]. What is relevant is that the Hamiltonian (120) has the form \( \tilde{H} = \tilde{H}_1(p) + \tilde{H}_2(x) \rightarrow H_1(\Pi) + H_2(\Phi) \), 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. 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 (120), 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 9.

In order to use this representation the constant coefficients \( D_{mn} \) and \( \Gamma_{nn_1\ldots n_k} \) that appear in the Hamiltonian (120) need to be computed. Using scale transformations (C.2) and the renormalization group equation (C.1) they can all be expressed in terms of the integrals
\[ d_n = \int \frac{ds(x)}{dx} \frac{ds(x-n)}{dx} dx \quad -4 \leq n \leq 4 \]
(123)
\[ \gamma_{m,n,k} = \int s(x) s(x-m) s(x-n) s(x-k) dx \quad -4 \leq m,n,k \leq 4. \] (124)
These integrals for different values of \( m, n, k \) are related to each other by finite linear equations derived from the renormalization group equation (C.1) and the scale fixing condition (C.8). These linear systems can formally be solved in terms of the coefficients \( h_l \) (C.3). The coefficients \( d_n \) are rational numbers and can be found in the literature on wavelets [50]. To find the coefficients \( \gamma_{mnk} \) requires solving a system of 9^3 linear equations. This eliminates the need to evaluate fractal valued functions. Alternatively the integrals \( \gamma_{mnk} \) can be approximated by noting that the renormalization group equation (C.1) and the scale fixing condition (C.8) 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.

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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 (120) are retained. In this case the overlap coefficients that appear in the Hamiltonian are related to $d_n$ and $\gamma_{lmn}$ by

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

(125)

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

$$
\Gamma_{0000} = 0.9528539
\Gamma_{0001} = 0.0670946
\Gamma_{0011} = 0.0890895
\Gamma_{0111} = -0.1424536
D_{00} = 295.56
D_{01} = -356.105
D_{10} = D_{01}
D_{11} = D_{00},
$$

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

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

(126)

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.

$$H \rightarrow H_F.$$  

(127)

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:

\[
U_F(t) = e^{-iH_F t} = \lim_{N \to \infty} \left( e^{-iH_F(\Pi) \Delta t} e^{-iH_F(\Phi) \Delta t} \right)^N
\]  

(128)

where \( \Delta t = t/N \) and

\[
H_F = H_F(\Pi) + H_F(\Phi)
\]

with

\[
H_F(\Pi) := \frac{1}{2} \sum_n \Pi_n \Pi_n
\]

(130)

and

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

(131)

This 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 \( \phi_n, \pi_n = ne \) 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 \( \langle \phi | \chi \rangle = \chi(n_1 \epsilon, \cdots, n_F \epsilon) \) 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 discrete 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 \( P_\chi \) 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

\[
\langle n_1, n_2, \cdots, n_F | U_F(t) | \chi(0) \rangle = \lim_{N \to \infty} \langle n_1, n_2, \cdots, n_F | \left( e^{-iH_F(\Pi) \Delta t} e^{-iH_F(\Phi) \Delta t} \right)^N \rangle | \chi(0) \rangle.
\]

(132)

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:

\[
\int d\phi = e^F \sum_{n_1 = -K}^K \cdots \sum_{n_F = -K}^K.
\]

(133)
for vectors representing a value of the eigenvalues of each of the $F$ independent $\phi$ field modes,

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

(134)

for vectors representing the value of the eigenvalues of each of the $F$ independent $\pi$ field modes,

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

(135)

and

$$\gamma = (\phi_0, \phi_1, \cdots, \phi_N)$$

(136)

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 8:

$$P_X(\phi', \phi, \Delta t) := \sum_{n''} (\phi' | \pi'' \rangle e^{-i \pi'' \cdot \pi'' \Delta t} e^F \langle \pi | \phi \rangle e^F. \tag{137}$$

It follows from (B.4) that $P_X(\phi', \phi, \Delta t)$ has the property

$$\sum_n P_X(\phi', \phi, \Delta t) = 1 \tag{138}$$

and

$$P_X(\phi_1, \phi_N, \cdots, \phi_1) := P_X(\phi_1, \phi_N, \Delta t) P_X(\phi_N, \phi_{N-1}, \Delta t) \cdots P_X(\phi_3, \phi_2, \Delta t) P_X(\phi_2, \phi_1, \Delta t) \tag{139}$$

also satisfies

$$\sum_{\gamma \in \Gamma} P_X(\phi_1, \phi_N, \cdots, \phi_1) = 1. \tag{140}$$

Equation (139) 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 $e^F$ and only summing over $\phi_1$ gives the evolution due to free propagation

$$\langle \phi_1 | e^{-i \Pi \cdot \Pi} | \phi_1 \rangle = \sum_{n_0 \rightarrow n_1} P_X(\phi_1, \phi_N, \cdots, \phi_1) e^{-F}. \tag{141}$$

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

$$W[\gamma] := e^{i \sum_n H_F(\phi_n) \Delta t} \tag{142}$$

with respect to the complex probability distribution (140), 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
\[
\langle n_1, n_2, \ldots, n_F | U_F(t) | \chi(0) \rangle = \sum_{\gamma} P_X(\phi_f, \phi_N, \ldots, \phi_1) W[\gamma] \chi(\phi_1) \quad (143)
\]
where \(U_F(t)\) is the unitary time evolution operator (128) 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
\[
P_X(\phi_f, \phi_N, \ldots, \phi_1) W[\gamma] = X(\phi_f, \phi_N, \Delta t) e^{iH_F(\phi_N)\Delta t} X(\phi_N, \phi_{N-1}, \Delta t) e^{iH_F(\phi_{N-1})\Delta t} \ldots X(\phi_3, \phi_2, \Delta t) e^{iH_F(\phi_2)\Delta t} X(\phi_2, \phi_1, \Delta t) e^{iH_F(\phi_1)\Delta t}. \quad (144)
\]
This represents time evolution as the product of large approximate transfer matrices.

Each stage of the calculation uses finite mathematics. The use of the finite Weyl representation exactly preserves unitary 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 9 and 10 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
\[
\langle \phi_1, \phi_2 | \psi \rangle = N e^{-\sum_{\ell=0}^{2}(\phi_\ell - \langle \phi_\ell \rangle)^2/(4\delta_\ell^2)}. \quad (145)
\]
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.

11. Summary and conclusion

This paper discusses a complex probability interpretation of the real-time Feynman path integral for systems of a finite number of degrees of freedom. In this interpretation the dynamics is expressed as the expectation value of a functional of paths with respect to a complex probability on a sample space of cylinder sets of ‘paths’. This interpretation follows from the completeness relation and the Trotter product formula. The motivation is that the complex probability interpretation also gives a rigorous reinterpretation of the real-time path integral on infinite dimensional Hilbert spaces \[2–4\], while the treatment of real time evolution as a path integral is difficult to interpret due to the absence of a countably additive positive measure on the cylinder sets of paths. For systems with a finite number of degrees of freedom the complex probability interpretation is a natural way to understand quantum dynamics, and is closely related to how the dynamics is treated in quantum computers. 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 a discrete-valued function of a continuous time variable as a path. The complex probability interpretation follows by observing that a sequence of discrete eigenvalues at different time steps is a label for a sequence of transition amplitudes from a...
state at the $n$th time step to a state at the $(n+1)$th time step. 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. Many ‘paths’ contribute to a given cylinder set, since all possible transition amplitudes are allowed at intermediate times strictly between these successive time steps. The complex probability is the product of the probability amplitudes for a given sequence of steps, while sum of all of these amplitudes gives the transition amplitude for the transition from a given initial state to a final state. When this is summed over all final states the result is one (the inner product of the initial state with itself). With this interpretation the Trotter product formula expresses the dynamics as a random variable on this probability space. The result of the expectation value of this random variable with respect to the complex probability is exactly, \( \langle a | e^{-iHt} | a \rangle \), which is an entire function of $t$ for a $D \times D$ dimensional Hamiltonian $H$.

Computations of multi-particle scattering observables or quantum field theory observables are candidates of problems that might be solved with quantum computers. These problems are formulated in infinite dimensional Hilbert spaces. For Hamiltonians that are sums of non-commuting operators the path integral representation of real-time evolution provides a means for treating the non-commuting operators in the Hamiltonian without having to explicitly diagonalize the Hamiltonian.

Quantum computers have a finite number of qubits, which means that the dynamics must be approximated, where the approximate dynamics is formulated on a finite-dimensional Hilbert space. The treatment of Hamiltonians with non-commuting operators is due to the Trotter product formula. When it is used in the finite dimensional case paths are replaced by ordered sequences of discrete eigenvalues of discrete Weyl operators. Each finite sequence of discrete eigenvalues is associated with an ordered product of transition amplitudes.

While this is not yet a model for quantum computing, any Hamiltonian can be expressed as a polynomial in the discrete Weyl representation. The Trotter product formula expresses time evolution as the expectation value of a random variable on the space of sequences of eigenvalues complementary pairs of discrete Weyl operators with respect to the complex probability defined by the ordered product of transition amplitudes.

A property of the discrete Weyl representation is that if the dimension is factored into a product of prime numbers, the discrete Weyl representation can be factored into a tensor product of irreducible representations of prime dimension. If the dimension is a power of 2 (i.e. $2^N$) then the Hilbert space can be represented by $N$ qubits, and the Weyl operators acting on each qubit can be represented by pairs of Pauli matrices.

In this case the $2^N$ Weyl operators represent a set of $2^N$ qubit gates, which by construction are irreducible. Products of these gates can be used to build two qubit gates. A ‘quantum gate’ in the original Weyl representation is replaced by a product of gates in the qubit representation. While mathematically equivalent, the qubit representation is the natural representation for quantum devices. In both cases the complex probability interpretation remains unchanged.

An important property of the complex probability for finite dimensional Hilbert spaces is that it exactly factors into products of conditional probabilities at each time step. This factorization also applies to the dynamics which modifies the phase of the transition amplitude at each time step (see (87)). The phase modification at each time step is represented by a quantum circuit. The factorization is also an important computational simplification.

In the qubit representation the discrete intermediate states are labeled by the states of all qubits at each time step, while quantum circuits define the random variable associated with time evolution. The qubit representation is natural for quantum computations since the complementary operators, $U_i$ and $V_i$, act on single qubits. These operators are the irreducible building blocks in this representation. This representation is efficient for treating local operators.
that can be expressed in terms of a small number of qubit operators. The two examples with continuous spectra illustrate how the direct approach can be used to investigate convergence with respect to the number of time steps and resolution before passing to a qubit representation. Hamiltonians for many realistic systems act on infinite dimensional Hilbert spaces. In this work these systems are treated as limiting cases of large finite dimensional systems rather than finite dimensional truncations of infinite dimensional systems.

Discrete approximations of infinite dimensional systems are discussed in section 7. These approximations were used to demonstrate the application of the discrete formulation of the path integral to 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 section 9, based time-dependent scattering theory, illustrates some of the issues that need to be considered in future realistic treatments of scattering using quantum computers.

While the goal of scattering calculations is to compute sharp-momentum scattering amplitudes, time-dependent scattering requires strong limits, which means that the sharp-momentum states must be replaced by wave packets. In the discrete case there are normalizable sharp-momentum states, but they are not acceptable for scattering because the corresponding position states are completely delocalized, so the scattered particle can never get out of the range of the potential. In addition efficient calculations require paying careful attention to the range of the interaction and both the width the both the momentum and position wave packets, which cannot be controlled independently.

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 section 10 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 construction of the multi-resolution wavelet basis is discussed in appendix C. The calculations presented in section 10 use a severe truncation of a $\phi(x)^4$ field theory to two modes, but the calculation is completely non-perturbative. Realistic calculations are still a long way off.

**Data availability statement**

All data that support the findings of this study are included within the article (and any supplementary files).

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**Appendix A. 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 a $M$ dimensional complex Hilbert space $\mathcal{H}$. The eigenvectors of $X$ are a basis on $\mathcal{H}$:

$$X|m\rangle = x_m|m\rangle \quad m = 1, \ldots, M.$$  \hspace{1cm} (A.1)

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

$$U|m\rangle = |m+1\rangle \quad m < M \quad U|M\rangle = |1\rangle.$$  \hspace{1cm} (A.2)

The labels $m$ on the eigenvectors are treated as integers mod $M$ so 0 is identified with $M$, 1 with $M+1$ etc. Since $U^M = I$, 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:

$$\lambda = u_m = e^{i\pi m}$$  \hspace{1cm} (A.3)

with orthonormal eigenvectors $|u_m\rangle$:

$$U|u_m\rangle = u_m|u_m\rangle$$  \hspace{1cm} (A.4)

$$\langle u_m|u_n\rangle = \delta_{mn}.$$  \hspace{1cm} (A.5)

The normalization (A.5) 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

$$0 = (U^M - I) = \frac{1}{u_n} \left( U^M - I \right) = \left( \frac{U}{u_n} \right)^M - I = \left( \frac{U}{u_n} - I \right) \left( I + \frac{U}{u_n} + \left( \frac{U}{u_n} \right)^2 + \cdots + \left( \frac{U}{u_n} \right)^{M-1} \right).$$  \hspace{1cm} (A.6)

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

$$I + \frac{U}{u_n} + \left( \frac{U}{u_n} \right)^2 + \cdots \left( \frac{U}{u_n} \right)^{M-1} = c|u_n\rangle \langle u_n|$$  \hspace{1cm} (A.7)

for some constant $c$. Applying (A.7) 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 $U$

$$|u_n\rangle \langle u_n| = \frac{1}{M} \sum_{m=1}^{M} \left( \frac{U}{u_n} \right)^m = \frac{1}{M} \sum_{m=0}^{M-1} \left( \frac{U}{u_n} \right)^m.$$  \hspace{1cm} (A.8)
Using (A.8) it follows that
\[ \langle k | u_n \rangle \langle u_n | k \rangle = \frac{1}{M} \sum_{m=0}^{M-1} \left( \frac{U}{u_n} \right)^m \langle k | k + m \rangle \]
\[ = \frac{1}{M} \sum_{m=0}^{M-1} \left( \frac{1}{u_n} \right)^m \langle k | k + m \rangle \]
\[ = \frac{1}{M} \] \hspace{1cm} (A.9)

This means that for any \( k \) and \( n \) that
\[ |\langle k | u_n \rangle| = \frac{1}{\sqrt{M}}. \] \hspace{1cm} (A.10)

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
\[ \langle M | u_n \rangle = \langle u_n | M \rangle = \frac{1}{\sqrt{M}}. \] \hspace{1cm} (A.11)

It follows from (A.11) and (A.8) that
\[ \langle k | u_n \rangle \langle u_n | M \rangle = \langle k | u_n \rangle \frac{1}{\sqrt{M}} = \frac{1}{M} \langle k | \sum_{m=1}^{M} u_n^{-m} | m \rangle = \frac{1}{M} u_n^{-k} \]
\[ = \frac{1}{M} e^{-2\pi i nk/M}. \] \hspace{1cm} (A.12)

Multiplying (A.12) by \( \sqrt{M} \) shows that the phase convention (A.11) fixes the inner product \( \langle k | u_n \rangle \) for all \( k \neq M \):
\[ \langle k | u_n \rangle = \frac{1}{\sqrt{M}} e^{-i \frac{2\pi nk}{M}}. \] \hspace{1cm} (A.13)

Schwinger defines another unitary operator, \( V \), that shifts the eigenvectors of \( U \) cyclically, but in the opposite direction
\[ V | u_n \rangle = | u_{n-1} \rangle, \quad n \neq 1, \quad V | u_1 \rangle = | u_M \rangle. \] \hspace{1cm} (A.14)

The same method, with \( U \) replaced by \( V \), gives
\[ V^M = I \] \hspace{1cm} (A.15)
\[ V | v_m \rangle = v_m | v_m \rangle, \quad v_m = e^{\frac{2\pi i m}{M}} \] \hspace{1cm} (A.16)
\[ |v_n\rangle \langle v_n| = \frac{1}{M} \sum_{m=0}^{M-1} \left( \frac{V}{v_n} \right)^m = \frac{1}{M} \sum_{m=1}^{M} \left( \frac{V}{v_n} \right)^m \] \hspace{1cm} (A.17)
and for unit normalized $|v_n\rangle$

$$|\langle u_k|v_n\rangle| = \frac{1}{\sqrt{M}}.$$  \hfill (A.18)

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

$$\langle u_M|v_n\rangle = \frac{1}{\sqrt{M}}.$$  \hfill (A.19)

Then (A.17) and the orthonormality of the $|u_k\rangle$'s give

$$\langle u_M|v_n\rangle\langle v_n|u_k\rangle = \langle u_k|v_n\rangle = \frac{1}{M}\sum_{m=0}^{M-1} e^{i\frac{2\pi}{M} m} |u_m\rangle \langle u_m|v_n\rangle = \frac{1}{M} v_n^{m-k}.$$  \hfill (A.20)

Multiplying (A.20) by $\sqrt{M}$ gives

$$\langle v_k|u_n\rangle = \frac{1}{\sqrt{M}} e^{-i\frac{2\pi}{M} m}.$$  \hfill (A.21)

Comparing (A.13) and (A.21) it follows that

$$|v_k\rangle = \sum_{m=0}^{M-1} |u_m\rangle \langle u_m|v_k\rangle = \sum_{m=0}^{M-1} e^{i\frac{2\pi}{M} m} |u_m\rangle \langle u_m|v_k\rangle = \sum_{m=0}^{M-1} \frac{1}{M} \sum_{m=0}^{M-1} e^{i\frac{2\pi}{M} m} |u_m\rangle \langle u_m|k\rangle = |k\rangle,$$  \hfill (A.22)

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

The spectral expansion of $V$, the identification (A.22) of $|v_k\rangle$ with $|k\rangle$ and the definition (A.2) of $U$ imply that the unitary operators $U$ and $V$ satisfy

$$UV = U \sum_{m=0}^{M-1} |v_m\rangle e^{i\frac{2\pi}{M} m} \langle v_m| = \sum_{m=0}^{M-1} |v_{m+1}\rangle e^{i\frac{2\pi}{M} m} \langle v_{m+1}| = \sum_{m=0}^{M-1} |v_{m+1}\rangle e^{i\frac{2\pi}{M} m} \langle v_{m+1}|U$$

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

$$= e^{-i\frac{\pi}{M}} VU.$$  \hfill (A.23)

$U$ 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 (A.2) give $U^{m-k}|v_k\rangle = |v_m\rangle$. When $m - k$ is negative the operator is either the $(k - m)$th power of the inverse (adjoint) of $U$ or equivalently it can be replaced by $M + m - k$ since $UM = I$. This also applies to the equations that follow. Using this with (A.17) gives

$$|v_m\rangle \langle v_k| = U^{m-k} |v_k\rangle \langle v_k| = \frac{1}{M} \sum_{n=0}^{M-1} e^{-i\frac{2\pi}{M} n} U^{m-k} V^n.$$  \hfill (A.24)
The order of the $U$ and $V$ operators can be changed using multiple applications of (A.23):

$$U^m V^n = U^{m-1} V^n U^{e^{-i2\pi n/M}} = U^{m-2} V^n U^{e^{-i2\pi (n+1)/M}} = \ldots = V^n U^m e^{-i2\pi n/M}. \quad (A.25)$$

Using (A.25) in (A.24) gives

$$\langle v_m | \langle v_k | O = \sum_{n=0}^{M-1} e^{-i\frac{2\pi n}{M}} V^n U^{m-k} e^{-i\frac{2\pi (m-k)}{M}} = \sum_{n=0}^{M-1} e^{-i\frac{2\pi n}{M}} V^n U^{m-k}. \quad (A.26)$$

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

$$O = \sum_{m,k=0}^{M-1} |v_m\rangle \langle v_m| O |v_k\rangle \langle v_k| = \sum_{m,k=0}^{M-1} \langle v_m| O |v_k\rangle |v_m\rangle \langle v_k|$$

$$= \frac{1}{M} \sum_{m,n,k=0}^{M-1} e^{-i\frac{2\pi n}{M}} \langle v_m| O |v_k\rangle U^{m-n} V^n$$

$$= \frac{1}{M} \sum_{m,n,k=0}^{M-1} e^{-i\frac{2\pi n}{M}} \langle v_m| O |v_k\rangle V^n U^{m-k}. \quad (A.27)$$

These equations have the form

$$O = \sum_{m,n=0}^{M-1} c_{mn} U^m V^n = \sum_{m,n=0}^{M-1} d_{mn} V^n U^m \quad (A.28)$$

which is the discrete Weyl representation of $O$. If $O$ commutes with $U$ then, using (A.25),

$$0 = \sum_{m,n=0}^{M-1} c_{mn} [U^m V^n, U] = \sum_{m,n=0}^{M-1} c_{mn} U^{m+1} V^n e^{i\frac{2\pi n}{M}} - 1 \quad (A.29)$$

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.

**Appendix B. Hamiltonians that are sums of non commuting operators**

The formalism discussed in (4) 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, eliminating $\tilde{H}_1(p)$, resulting in a complex probability on a space of ‘paths’ in the coordinate variable, $X$. As in the phase space case, these ‘paths’ have discrete values, so they are generally nowhere continuous.
In this case
\[\sum_n \langle k|\bar{n}\rangle \langle \bar{n}|H|m\rangle = \sum_n \langle k|\bar{n}\rangle \langle \bar{n}|m\rangle (H_1(p_n) + H_2(x_m)) = \sum_n \langle k|\bar{n}\rangle \langle \bar{n}|m\rangle \bar{H}_{nm}\]  
(B.1)

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

A new complex probability can be defined by
\[P_X(k_f;k_N,\ldots,k_1) := e^{i\bar{H}_1(p_n)} \sum_{n_1=0}^{N} \sum_{k_1=0}^{M-1} P(k_f,n_N,k_N,\ldots,n_1,k_1) e^{-i \sum \bar{H}_1(p_n) \Delta t}.\]  
(B.2)

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 \(k_3 \cdots k_N\) sums are just expressions for the identity. After eliminating \(k_3 \cdots k_N\) 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:
\[\sum_{n_1=0}^{N} \sum_{k_1=0}^{M-1} P(k_f,n_N,k_N,\ldots,n_1,k_1) e^{-i \sum \bar{H}_1(p_n) \Delta t} = \sum_{k_1=0}^{M-1} (k_f|\bar{n}) e^{-i \sum \bar{H}_1(p_n) \Delta t} (\bar{n}|k_1).\]

The \(k_1\) sum can be evaluated using
\[\sum_{n=0}^{M-1} (k_f|\bar{n}) e^{-i \sum \bar{H}_1(p_n) \Delta t} (\bar{n}|k_1) = \frac{1}{M} \sum_{n=0}^{M-1} e^{-i \pi n/M} \sum_{k_1=0}^{M-1} e^{i 2\pi k_1 n/M} e^{-i \bar{H}_1(p_n) \Delta t}\]
\[= \frac{1}{M} \sum_{n=0}^{M-1} e^{-i \pi n/M} e^{-i \bar{H}_1(p_n) \Delta t}\]
\[\times \left\{ (1 - e^{i 2\pi n/M}) = 0 \quad 1 < n < M - 1 \right.\]
\[\left. n = 0 \right\} = e^{-i \bar{H}_1(p_n) \Delta t}.\]  
(B.3)

Including the factor \(e^{i \bar{H}_1(p_n) \Delta t}\) gives
\[\sum_{k_f} P_X(k_f,k_N,\ldots,k_1) = e^{i \bar{H}_1(p_n) \Delta t} \sum_{n=0}^{M-1} \sum_{k_1=0}^{M-1} P(k_f,n_N,k_N,\ldots,n_1,k_1) e^{-i \sum \bar{H}_1(p_n) \Delta t} = 1.\]  
(B.4)

The expression for the evolution operator becomes
\[\langle k_f|e^{-i \bar{H}_1} |k_1\rangle = \sum_{k_f} P_X(k_f,k_N,\ldots,k_1) e^{-i \sum \bar{H}_1(x_m) \Delta t}\delta_{k_1,k_f}\]  
(B.5)

which is expressed as the expectation value of the functional \(e^{-i \sum \bar{H}_1(x_m) \Delta t}\) 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
\[P_X(k_{n+1};k_n) = \sum_m P(k_{n+1};m,k_n) e^{-i (\bar{H}_1(p_n) - \bar{H}_1(p_0)) \Delta t}.\]  
(B.6)
giving

\[ \langle k_f | e^{-iHt} | k_i \rangle = \lim_{N \to \infty} \sum_{X} \left( \prod_{n} P_{X}(k_{n+1}; k_{n}) e^{-t \sum \tilde{R}_{n} \Delta t} \right) \delta_{k_{1},k_{i}} \quad k_{f} = k_{N+1} \]  

(B.7)

which has the structure of the \( N \)th power of a \( M \times M \) matrix. In this discrete case the result becomes exact in the Trotter limit.

**Appendix C. Wavelet basis**

The construction of the wavelet basis used to construct the discrete representation of the Hamiltonian (120) is outlined below. The starting point the solution of the linear renormalization group Equation

\[ s(x) = \sum_{l=0}^{2L-1} h_l D f(x) \]  

(C.1)

where

\[ D f(x) := \sqrt{2} f(2x) \quad \text{and} \quad T f(x) := f(x - 1) \]  

(C.2)

are unitary discrete dyadic scale transformations and unit translations. Here \( L \) is a positive integer that determines the type of Daubechics’s wavelets. 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 choice is \( L = 3 \) where the solution \( s(x) \) of (C.1), 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

\[ h_0 = \left( 1 + \sqrt{10} + \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2} \]

\[ h_1 = \left( 5 + \sqrt{10} + 3 \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2} \]

\[ h_2 = \left( 10 - 2 \sqrt{10} + 2 \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2} \]

\[ h_3 = \left( 10 - 2 \sqrt{10} - 2 \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2} \]

\[ h_4 = \left( 5 + \sqrt{10} - 3 \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2} \]

\[ h_5 = \left( 1 + \sqrt{10} - \sqrt{5 + 2 \sqrt{10}} \right) / 16\sqrt{2}. \]  

(C.3)
They are determined by the requirement that the solution of (C.1) satisfies

\begin{equation}
\sum_{l=0}^{2L-1} h_l = \sqrt{2} \tag{C.4}
\end{equation}

\begin{equation}
\int s_m(x) s_0(x) \, dx = \delta_{m0} \tag{C.5}
\end{equation}

and

\begin{equation}
x^k = \sum_{n=-\infty}^{\infty} c_n s(x-n) \quad 0 \leq k \leq L. \tag{C.6}
\end{equation}

These become equations for the \( h_l \) when (C.1) is used in (C.4)–(C.6). Equation (C.5) means that integer translates of \( s(x) \) are orthonormal while (C.6) means that locally finite linear combinations of \( s_n(x) = s(x-n) \) can pointwise represent low degree polynomials.

Given the solution, \( s(x) \), of (C.1) new functions are constructed from \( s(x) \) by rescaling and translating

\begin{equation}
s_k^N(x) := D^k T^N(x) s(x) = \sqrt{2^k} s(2^k x - n). \tag{C.7}
\end{equation}

Since (C.1) is homogeneous in \( s(x) \) the starting scale can be fixed by requiring

\begin{equation}
\int s(x) \, dx = 1. \tag{C.8}
\end{equation}

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

\begin{equation}
\mathcal{S}^k := \left\{ f(x) | f(x) = \sum_{n=-\infty}^{\infty} c_n s_k^N(x) \quad \sum_{n=-\infty}^{\infty} |c_n|^2 < \infty \right\}. \tag{C.9}
\end{equation}

The renormalization group equation (C.1) implies

\begin{equation}
\mathcal{S}^k \subset \mathcal{S}^{k+1}. \tag{C.10}
\end{equation}

It follows that

\begin{equation}
\mathcal{S}^{k+1} = \mathcal{S}^k \oplus \mathcal{W}^k, \tag{C.11}
\end{equation}

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’:

\begin{equation}
w_k^N(x) = D^k T^N w(x) \tag{C.12}
\end{equation}

where

\begin{equation}
w(x) := \sum_{l=0}^{2L-1} (-1)^l h_{2L-1-l} D^l s(x) \tag{C.13}
\end{equation}
is called the ‘mother wavelet’. This decomposition can be continued to generate a multi-resolution decomposition of $L^2(\mathbb{R})$

$$L^2(\mathbb{R}) = s^k \oplus \bigoplus_{l=0}^{\infty} W^{k+l}. \quad (C.14)$$

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

$$\{\xi_n(x)\}_{n=-\infty}^{\infty} = \{s_n^k(x)\}_{n=-\infty}^{\infty} \cup \{w_n^l(x)\}_{n=-\infty, l=k}^{\infty}. \quad (C.15)$$

For the choice $L = 3$ the basis functions $s_n^k(x)$ and $w_n^l(x)$ have compact support on $[2^{-k}n, 2^{-k}(n+5)]$. All of the basis functions have one continuous derivative so the coefficients (121) 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.

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