Path integrals and the discrete Weyl representation

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Abstract

This paper uses Schwinger's representation of quantum systems of a finite number of degrees of freedom to formulate discrete path integral representations of the dynamics. The representation starts with an observable with a finite number of distinct eigenvalues. Using that observable Schwinger constructs complementary pairs of finite dimensional unitary operators that are finite dimensional analogs of the irreducible Weyl algebra. These can be decomposed into products of irreducible sub-algebras that reduce to q-bit gates for the case of 2^N degrees of freedom. In the limit of a large number of discrete degrees of freedom these representations can be used to model quantum systems with continuous degrees of freedom. This limit recovers the continuum Weyl algebra. Path integrals can be formulated in the discrete case. They have the advantage that the number of paths for a finite number of time slices is finite. In this work the path integral is interpreted as the expectation value of a potential functional with respect to a complex probability distribution on the space of "paths". An application to scattering from a short-range potential is given. Multi-resolution wavelet bases are used exactly represent a local $\phi^4(x)$ quantum field theory as a theory with an infinite number of discrete local modes. The discrete path integral is illustrated by computing time evolution when this theory is truncated to two coupled modes.

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I. INTRODUCTION

Quantum computers consist of a finite number, M, of two state systems. The resulting Hilbert space for this quantum system is finite dimensional. Elementary gates are used to build an irreducible algebra of operators on this space that can be used to model complex systems. The goal is to time evolve these systems to solve problems that are difficult to solve classically. This requires time evolving vectors with large numbers of components and measuring the results. At the computational level results are achieved using finite quantum systems. Julian Schwinger's textbook [1] treatment of measurement theory generalizes the standard measurement theoretic treatment of the Stern Gerlach experiment to a system of a finite number of degrees of freedom. It is a natural framework for numerical treatments of path integrals, although these applications are limited on classical computers. Schwinger begins with a quantum observable that has a finite number of possible outcomes. He then constructs a complementary set of unitary operators - one that has the same eigenvectors as the original observable and one that cyclically shifts the eigenvectors. These two unitary operators are finite degree of freedom analogs of the Weyl algebra, which is the exponential form of the canonical commutation relations. In this case there is no identification of these observables with coordinates or momenta. When M can be expressed as a product of prime factors, he shows that this algebra can be decomposed into products of irreducible subalgebras acting on independent sets of prime numbers of degrees of freedom. When $M = 2^L$ these elementary unitary operators can be represented by the q-bit gates σ_x and σ_z.

While Schwinger's representation provides a general structure theorem for quantum systems of a finite numbers of degrees of freedom, there are natural limits that provide models of quantum systems based on commuting observables with continuous eigenvalues. These systems can be approximated by finite systems with large number of degrees of freedom. The discrete representation leads to a discrete formulation of the path integral where for N time steps there are a finite number, M^N, "paths" that pass through the M allowed values of one of the observables at each time step. For a canonical system that is quadratic in the "momentum" variables, the amplitude for free propagation between time steps defines a "complex probability" on the space of paths. The path integral can be interpreted as the small time step limit of the expectation value of an interaction functional of the discrete of paths between time steps. An application of this discrete path integral to scattering in one

dimension is illustrated in section VIII. The discrete path integral is used to approximate sharp-momentum half-shell transition matrix elements. The same method can be applied to time evolve quantum fields using an exact discrete multi-resolution representation of the field algebra. The computation of time evolution of a volume and resolution truncated quantum field theory using the discrete path integral is discussed in section IX. It is illustrated using a trivial two mode truncation of the theory.

While the Schwinger representation does not solve any of the problems that quantum computers are designed to solve, it leads to a simple framework for modeling general quantum problems as finite quantum systems, where these finite systems can also be represented by products of elementary 2 or 3 state quantum systems. The 2-3 state algebras are more localized and should provide a more practical representation for quantum computations. In general applications are limited by the dimension of the vectors that represent realistic systems.

The next section provides a brief discussion of the role of Hilbert spaces in the formulation of three valued quantum logic represented by q-bits. This emphasizes the relevant difference between digital and quantum computing. Section III provides a summary of Schwinger's construction of irreducible algebras of systems of M degrees of freedom. Section IV discusses the factorization of a 2^M degree of freedom system into a direct product of irreducible two-degree of freedom systems which results in a representation of the algebra of section III in terms of qbits. Section V discusses the limit to a system with continuous eigenvalues. In this case the general construction requires additional boundary conditions. Section VI gives a short discussion of the subject of complex probabilities, which will be used in the discrete formulation of the path integral. Section VII discusses the treatment of time evolution using a discrete formulation of the path integral as the expectation value of a potential functional with respect to a complex probability on a finite sample space of paths. Section VIII illustrates the application of the path integral in section VII to scattering in one dimension. Section IX discusses an exact discrete multi-resolution representation of a scalar field theory and uses the path integral in section VII to time evolve a two field-mode truncation of the theory. Section X gives a summary and conclusion.

II. QUANTUM LOGIC

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

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

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

$$P_{ab} := \frac{\langle a|b\rangle\langle b|a\rangle}{\langle a|a\rangle\langle b|b\rangle}$$

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

$$(1) \qquad P_{ab} = 1 \qquad (2) \qquad P_{ab} = 0 \qquad (3) \qquad 0 < P_{ab} < 1. \tag{1}$$

When the Hilbert space is two dimensional the difference in these two types of logic is encoded in bits or q-bits respectively.

In quantum mechanics observable quantities are represented by linear operators A on a Hilbert space. The only possible outcomes for measuring A are one of its eigenvalues, a_n (this assumes A is a normal operator whose eigenvectors form a basis). In this case the Hilbert space has a decomposition $\mathcal{H} = \oplus_n \mathcal{H}_n$, where the $\mathcal{H}_n$ are A-invariant subspaces of $\mathcal{H}$.

The mean value of a measurement of A in state $|b\rangle$ is

$$\langle b|A|b\rangle = \sum_n P_{a_n b} a_n \qquad a_n \text{ eigenvalue of A} \tag{2}$$

which is the weighted average of the quantum probabilities for a measurement of b to be in one of the eigenstates of A.

III. SCHWINGER'S DISCRETE WEYL ALGEBRA

This section reviews Schwinger's [1] 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 quantum system. This construction is essentially the same as the treatment of the quantum Fourier transform discussed in [3] and elsewhere.

Let $\mathcal{H}$ be a M-dimensional complex Hilbert space. Let A be a normal operator on $\mathcal{H}$ with M distinct eigenvalues and unit normalized eigenvectors:

$$A|a_m\rangle = a_m|a_m\rangle \qquad m = 1, \cdots, M \qquad a_m \neq a_n \text{ for } m \neq n. \tag{3}$$

Define the operator U on $\mathcal{H}$ that cyclically shifts the eigenvectors of A:

$$U|a_m\rangle = |a_{m+1}\rangle \qquad m < M \qquad U|a_M\rangle = |a_1\rangle. \tag{4}$$

In what follows the labels m on eigenvectors and eigenvalues are treated as integers mod M so 0 is identified with M, 1 with $M+1$ etc.. U defined by (4) is unitary since

$$UU^\dagger = \sum_{m=1}^{M} U|a_m\rangle\langle a_m|U^\dagger = \sum_{m=1}^{M-1} |a_{m+1}\rangle\langle a_{m+1}| + |a_1\rangle\langle a_1| = \sum_{m'=1}^{M} |a_{m'}\rangle\langle a_{m'}| = I. \tag{5}$$

Since M applications of U leaves all M basis vectors, $|a_m\rangle$, unchanged, it follows that $U^M = I$. This means that the characteristic polynomial of U is $P(\lambda) = \lambda^M - 1 = 0$. The eigenvalues of U are the M roots of 1:

$$\lambda = u_m = e^{\frac{2\pi m i}{M}}. \tag{6}$$

Let $|u_m\rangle$ denote the associated eigenvectors:

$$U|u_m\rangle = u_m|u_m\rangle \tag{7}$$

with unit normalization

$$\langle u_m|u_n\rangle = \delta_{mn}. \tag{8}$$

The normalization does not fix the phase which will be fixed later. Since both $U^M = I$ and $u_n^M = 1$ it follows that

$$0 = (U^M - I) = \frac{1}{u_n^M}(U^M - I) =$$

$$\left((\frac{U}{u_n})^M - I\right) = \prod_{m=1}^{M}(\frac{U}{u_n} - \frac{u_m}{u_n}) = (\frac{U}{u_n} - 1)(1 + \frac{U}{u_n} + (\frac{U}{u_n})^2 + \cdots + (\frac{U}{u_n})^{M-1}). \quad (9)$$

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

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

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

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

Using (11) it follows that

$$\langle a_k|u_n\rangle\langle u_n|a_k\rangle = \frac{1}{M}\sum_{m=0}^{M-1}\langle a_k|(\frac{U}{u_n})^m|a_k\rangle = \frac{1}{M}\sum_{m=0}^{M-1}(\frac{1}{u_n})^m\langle a_k|a_{k+m}\rangle = \frac{1}{M}. \quad (12)$$

This means for any k and n that

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

The interpretation is that if the system is prepared in any eigenstate of U and A is subsequently measured, then the probability of measuring any of the eigenvalues of A 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 A. This is the condition for the observables A and U to be complementary.

The phase of $|u_n\rangle$ is defined by choosing

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

It then follows from (14) that

$$\langle a_k|u_n\rangle\langle u_n|a_M\rangle = \langle a_k|u_n\rangle\frac{1}{\sqrt{M}} =$$

$$\frac{1}{M}\langle a_k|\sum_{m=1}^{M}u_n^{-m}|a_m\rangle = \frac{1}{M}u_n^{-k} = \frac{1}{M}e^{-2\pi ink/M} \quad (15)$$

which gives the inner product

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

Next define another unitary operator, V, that shifts the eigenvectors of U cyclically, but in the opposite direction

$$V|u_n\rangle = |u_{n-1}\rangle, \qquad n \neq 1, \qquad V|u_1\rangle = |u_M\rangle. \tag{17}$$

The same methods, with U replaced by V, give

$$V^M = I \tag{18}$$

$$V|v_m\rangle = v_m|v_m\rangle \qquad v_m = e^{\frac{2\pi i m}{M}} \tag{19}$$

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

and for unit normalized $|v_n\rangle$

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

The phase of the $|v_n\rangle$ is defined by choosing

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

With this choice of phase

$$\langle u_M|v_n\rangle\langle v_n|u_k\rangle = \langle v_n|u_k\rangle\frac{1}{\sqrt{M}} = \frac{1}{M}\sum_{m=0}^{M-1} v_n^{-m}\langle u_m|u_k\rangle = \frac{1}{M}v_n^{-k} \tag{23}$$

which gives

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

Comparing (16) and (24) it follows that

$$|v_k\rangle = \sum_{m=0}^{M-1}|u_m\rangle\langle u_m|v_k\rangle = \sum_{m=0}^{M-1}|u_m\rangle\frac{e^{2\pi ink/M}}{\sqrt{M}} = \sum_{m=0}^{M-1}|u_m\rangle\langle u_m|a_k\rangle = |a_k\rangle \tag{25}$$

so the operators A and V have the same eigenvectors. The unitary operators U and V defined above satisfy

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

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

or

$$\boxed{UV = VUe^{\frac{-2\pi i}{M}}.} \tag{27}$$

U and V form an irreducible set of operators in the sense that that any operator on the Hilbert space can be expressed as a degree $(M-1)\times(M-1)$ polynomial these two operators. To show this note

$$|v_m\rangle\langle v_k| = U^{m-k}|v_k\rangle\langle v_k| =$$

$$\frac{1}{M}\sum_{n=0}^{M-1} e^{-2\pi ink/M}U^{m-k}V^n = \frac{1}{M}\sum_{n=0}^{M-1} e^{-2\pi imn/M}V^nU^{m-k} \tag{28}$$

where (27) was used to change the order of the U and V operators in (28). Irreducibility follows since a general operator O can be expressed in terms of its matrix elements in a basis

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

$$\frac{1}{M}\sum_{m,n,k=0}^{M-1} e^{-2\pi ink/M}\langle v_m|O|v_k\rangle U^{m-k}V^n = \frac{1}{M}\sum_{m,n,k=0}^{M-1} e^{-2\pi imn/M}\langle v_m|O|v_k\rangle V^nU^{m-k}. \tag{29}$$

These equations have the form

$$\boxed{O = \sum_{m,n=0}^{M-1} a_{mn}U^mV^n = \sum_{m,n=0}^{M-1} b_{mn}V^mU^n} \tag{30}$$

which is the Weyl representation of O. If O commutes with U then

$$0 = \sum_{mn=0}^{M-1} a_{mn}[U^mV^n, U] = \sum_{mnk=0}^{M-1} a_{mn}U^{m+1}V^n(e^{2\pi in/M} - 1) \tag{31}$$

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. This means that any operator that commutes with both U and V is a constant multiple of the identity.

The following property will be used in the discussion of complex probabilities

$$\boxed{\sum_{m=0}^{M-1}\langle u_n|v_m\rangle = \frac{1}{\sqrt{M}}\sum_{m=0}^{M-1} e^{\frac{2\pi imn}{M}} = \delta_{n0}\sqrt{M} = \delta_{nM}\sqrt{M}}. \tag{32}$$

To prove this consider two cases. If $n = 0$ or M the sum is M. Otherwise

$$\sum_{m=0}^{M-1} e^{\frac{2\pi imn}{M}} = \frac{1 - e^{2\pi in}}{1 - e^{2\pi in/M}} = 0 \qquad 0 < n < M. \tag{33}$$

IV. QBITS

One property of the Schwinger representation is that it has a natural representation in terms of q-bits. When M can be factored into products of prime numbers the U and V 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 a product of q-bit gates.

To show this assume that $M = 2^L$ 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: $n \leftrightarrow (n_1, n_2, \cdots, n_L)$

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

This results in the identifications

$$|u_{n_1 \cdots n_L}\rangle := |u_n\rangle \qquad |v_{n_1 \cdots n_L}\rangle := |v_n\rangle. \tag{35}$$

Define unitary operators U_i and V_i by

$$U_i |v_{n_1 \cdots n_L}\rangle = |v_{n_1 \cdots [n_i+1]_{\mathrm{mod}\, 2} \cdots n_L}\rangle \tag{36}$$

$$V_i |u_{n_1 \cdots n_L}\rangle = |u_{n_1 \cdots [n_i-1]_{\mathrm{mod}\, 2} \cdots n_L}\rangle. \tag{37}$$

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

$$U_i^2 - 1 = V_i^2 - 1 = 0, \tag{38}$$

$$[U_i, U_j] = [V_i, V_j] = 0 \qquad [U_i, V_j] = 0 \qquad i \neq j \qquad V_i U_i = U_i V_i e^{i\pi} \tag{39}$$

$$U^n = \prod_{m=1}^{L} U_m^{n_m} \tag{40}$$

$$V^n = \prod_{m=1}^{L} V_m^{n_m}. \tag{41}$$

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 simple matrix representation of U_i and V_i is

$$V_i = \sigma_3 \qquad U_i = \sigma_1 \tag{42}$$

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

$$|v_0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |v_1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{43}$$

$$|u_0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |u_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{44}$$

The operators σ_1 and σ_3

$$U_i = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad V_i = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{45}$$

satisfy (4) and (17) for $M = 2$. They also satisfy

$$\sigma_3\sigma_1 = \sigma_1\sigma_3 e^{\frac{2\pi i}{2}} \qquad (\sigma_1^2 - 1) = (\sigma_3^2 - 1) = 0. \tag{46}$$

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

$$A = a_1 I + a_2\sigma_1 + a_3\sigma_3 + a_4\sigma_3\sigma_1. \tag{47}$$

This shows how the discrete version of the irreducible Weyl algebra can be built up out of q-bits using the two elementary gates σ_1 and σ_3 acting on each qbit. This means that any operator on the 2^L dimensional Hilbert space can be expressed as a polynomial in the L pairs of 2 state U and V operators.

Note for M odd the same construction works with 3×3 matrices with

$$U_i = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad V_i = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{2\pi i/3} & 0 \\ 0 & 0 & e^{4\pi i/3} \end{pmatrix}. \tag{48}$$

V. SCHWINGER'S CONTINUUM LIMIT

The eigenvalue spectrum of many observables of interest, like momenta and coordinates, are continuous. 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. To do this assume M is large and define the small quantity ϵ by

$$\epsilon^2 := 2\pi/M. \tag{49}$$

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

$$p_l = l\epsilon = l\sqrt{\frac{2\pi}{M}} \qquad q_l = l\epsilon = l\sqrt{\frac{2\pi}{M}} \qquad -K\epsilon \leq q_l, p_l \leq K\epsilon \tag{50}$$

where

$$K\epsilon = \sqrt{\frac{M\pi}{2}} - \sqrt{\frac{\pi}{2M}}. \tag{51}$$

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

While for finite M any vector with finite 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 U and V given by (4) and (17) Hermitian operators $\hat{p}$ and $\hat{q}$ are defined by

$$\boxed{V = e^{i\epsilon\hat{p}} \qquad U = e^{i\epsilon\hat{q}}}. \tag{52}$$

These can be used to define

$$V(q_m) = e^{i\hat{p}q_m} = e^{i\hat{p}\epsilon m} = V^m \tag{53}$$

$$U(p_n) = e^{i\hat{q}p_n} = e^{i\hat{q}\epsilon n} = U^n. \tag{54}$$

With these definitions equation (27) becomes

$$V(q_m)U(p_k) = U(p_k)V(q_m)e^{\frac{i2\pi mk}{M}} = U(p_k)V(q_m)e^{i\epsilon m\epsilon k} = U(p_k)V(q_m)e^{ip_kq_m} \tag{55}$$

$$\boxed{V(q_m)U(p_k) = U(p_k)V(q_m)e^{ip_kq_m}} \tag{56}$$

which is the Weyl [4] form of the canonical commutation relations, where in this case the variables are discrete. Equations (53-54) motivate the definitions

$$dp = \epsilon dn = \sqrt{\frac{2\pi}{M}}dn \qquad dq = \epsilon dn = \sqrt{\frac{2\pi}{M}}dn. \tag{57}$$

It follows from (52) that eigenvectors of V are also eigenvectors of $\hat{p}$ and the eigenvectors of U are also eigenvectors of $\hat{q}$. Choosing normalization of the state $|p_n\rangle$ and $|q_n\rangle$ so

$$\int dp \approx \sum_{l=-K}^{K} \frac{dp}{dl} = \epsilon \sum_{l=-K}^{K} \qquad \int dq \approx \sum_{l=-K}^{K} \frac{dq}{dl} = \epsilon \sum_{l=-K}^{K} \tag{58}$$

$$I = \sum_{l=-K}^{K} |v_l\rangle\langle v_l| = \sum_{l=-K}^{K} |p_l\rangle dp_l \langle p_l| = \sum_{l=-K}^{K} |p_l\rangle \epsilon \langle p_l| \tag{59}$$

$$I = \sum_{l=-K}^{K} |u_l\rangle\langle u_l| = \sum_{l=-K}^{K} |q_l\rangle dq_l \langle q_l| = \sum_{l=-K}^{K} |q_l\rangle \epsilon \langle q_l| \tag{60}$$

and comparing these equations leads to the definitions

$$|p_l\rangle := |v_l\rangle/\sqrt{\epsilon} \tag{61}$$

and

$$|q_l\rangle := |u_l\rangle/\sqrt{\epsilon}. \tag{62}$$

Using these relations gives

$$\langle p_m|q_n\rangle = \frac{1}{\epsilon}\langle v_m|u_n\rangle = \frac{1}{\epsilon\sqrt{M}} e^{\frac{-2\pi imn}{M}} = \frac{1}{\sqrt{2\pi}} e^{-ip_m q_n} \tag{63}$$

$$\langle p_m|p_n\rangle = \frac{1}{\epsilon}\langle v_m|v_n\rangle = \frac{\delta_{mn}}{\epsilon} \tag{64}$$

and

$$\langle q_m|q_n\rangle = \frac{1}{\epsilon}\langle u_m|u_n\rangle = \frac{\delta_{mn}}{\epsilon}. \tag{65}$$

A result that will be used later to reinterpret the path integral as the expectation of a potential functional with respect to a complex probability distribution follows from (32). Consider the expression

$$\sum_{lm} \langle q_n|p_l\rangle dp_l f(p_l) \langle p_l|q_m\rangle dq_m = \frac{\epsilon^2}{2\pi} \sum_{l=-K}^{K} \sum_{m=-K}^{K} e^{i(q_n - q_m)p_l} f(p_l). \tag{66}$$

The m sum can be computed in closed form

$$\sum_{m=-K}^{K} e^{iq_m p_l} = \sum_{m=-K}^{K} e^{\frac{2\pi ml}{M}} = e^{\frac{-i\pi lK}{M}} \left(\frac{1}{1 - e^{\frac{2\pi l}{M}}} - \frac{e^{2\pi l}}{1 - e^{\frac{2\pi l}{M}}} \right) = \delta_{l0} M. \tag{67}$$

Using (67) in (66) with (49) gives

$$\boxed{\sum_{lm} \langle q_n|p_l\rangle dp_l f(p_l) \langle p_l|q_m\rangle dq_m = \frac{M\epsilon^2}{2\pi} f(0) = f(0).} \tag{68}$$

The same result is obtained by "integrating" over the final q_n instead of the initial q_m. This result will be used in the development of discrete path integrals that follows.

VI. 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

$$P(S_i) = \sum_{s \in S_i} P(s) \qquad P(S) = 1. \tag{69}$$

$P(S_i)$ is the complex probability assigned to the subset S_i of S. It follows that

$$P(S_i) + P(S_i^c) = 1 \tag{70}$$

where S_i^c is the complement of S_i in S, and for a finite set of non-intersecting subsets of S

$$S_i \cap S_j = \ i \neq j \qquad P(\cup S_i) = \sum_i P(S_i). \tag{71}$$

In the applications that follow the sample set will be a finite collection of paths.

More generally, since $P(s)$ is complex, equation (71) cannot be extended to countable non-intersecting subsets, which is where complex probabilities differ from ordinary probabilities [5][6]. This is not an issue for finite sample sets. The extension of the notion of complex probabilities to continuous a sample set generated from intervals by complements and finite unions, based on the Henstock integral [7][8][9], was used in [10][11] to prove that the real-time path integral formulated as the expectation of a potential functional with respect to a complex probability distribution on cylinder sets of paths converges to a global solution of the Schrödinger equation. This was applied to compute scattering amplitudes using real-time path integrals in a simple model in [12]. In that case the complex probability was a probability on a finite collection of cylinder sets rather than a discrete set of paths. To treat the large number of cylinder sets, the probability was approximately factored into products of one-step probabilities, which reduced the problem to computing powers of approximate transfer matrices. Because of the approximation unitarity was only preserved approximately. In the discrete case the sample set is finite, the complex probability exactly factors into a product of one time step complex probabilities and the transfer matrices associated with the one-step probabilities are exactly unitary.

A random variable $F(s)$ is a function on the sample set S with expectation value

$$E[F] = \sum_{s \in S} P(s)F(s).$$

In this paper the sample set is the finite collection of paths that have M possible values at each of N time steps, the complex probability, $P(s)$ is associated with free propagation through N time steps along the path "s", and $F(s)$ is the contribution from the potential due to the path "s". This is discussed in the next section.

VII. COMPLEX PROBABILITIES IN REAL TIME PATH INTEGRALS

The path integral for a system with one degree of freedom is formulated using the discrete representation discussed section III. Following references [6][10][11], the path integral will be defined as the expectation value of a potential functional with respect to a complex probability distribution.

To do this it is necessary to:

1.) Define the space of paths

2.) Define complex probabilities on the space of paths

3.) Identify the path integral with the expectation value of a functional on the space of paths.

Let H be a canonical Hamiltonian with one degree of freedom of the form

$$H = \frac{\hat{p}^2}{2\mu} + V(\hat{q}) \tag{72}$$

where $\hat{q}$ and $\hat{p}$ are canonically conjugate operators satisfying

$$[\hat{q}, \hat{p}] = i. \tag{73}$$

The starting point for constructing a path integral is the Trotter product formula [13][14]:

$$\langle q_f, t_f | e^{-iHt} | q_i, t_i \rangle = \langle q_f, t_f | (e^{-iHt/N})^N | q_i, t_i \rangle =$$

$$\lim_{N\to\infty} \langle q_f, t_f | (e^{-iHt/N})^N | q_i, t_i \rangle = \lim_{N\to\infty} \langle q_f, t_f | (e^{-i(\hat{p}^2/2\mu)\Delta t} e^{-iV(\hat{q})\Delta t})^N | q_i, t_i \rangle \tag{74}$$

where $\Delta t := t/N$. This is the operator generalization of the representation

$$e^x = \lim_{N\to\infty} (1 + \frac{x}{N})^N \tag{75}$$

of e^x. Equation (74) is exact in the limit that $N \to \infty$ when applied to a normalizable wave packet. It is also possible to express $e^{-iH\Delta t}$ in terms of the U and V operators in the Weyl representation (30), however the more familiar representations are used in this section.

Following the standard steps in evaluating the path integrals, sums over complete sets of eigenstates of U and V are inserted between the operators in (74):

$$\langle q_f|e^{-iHt}|\psi\rangle = \int \langle q_f|e^{-iHt}|q_i\rangle dq_i \psi(q_i) dq_i =$$

$$\lim_{N\to\infty} \int \langle q_f|p_N\rangle dp_N e^{-i(p_N^2/2\mu)\Delta t} \langle p_N|q_N\rangle dq_N e^{-iV(q_N)\Delta t} \cdots$$
$$\cdots \langle q_2|p_1\rangle dp_1 e^{-i(p_1^2/2\mu)\Delta t} \langle p_1|q_1\rangle dq_1 \langle q_1|e^{-iV(q_1)\Delta t}|\psi\rangle. \tag{76}$$

The next step is to approximate the integrals by numerical quadratures. This is done using the discrete variables introduced in the previous section. While this is not the most efficient approximation, it has the advantage that everything is discrete, finite and exactly unitary.

In this case for an N time step Trotter approximation the discrete variable q_i for the i-th time step can take on the $2K+1$ discrete values $l\epsilon$, $-K \le l \le K$ and the transition amplitude (76) becomes

$$\langle q_f|e^{-iH(t)}|\psi\rangle \approx \sum \langle q_f|p_{Nn_N}\rangle \epsilon e^{-i(p_{Nn_N}^2/2\mu)\Delta t} \langle p_{Nn_N}|q_{Nn_N}\rangle \epsilon e^{-iV(q_{Nn_N})\Delta t} \times$$
$$\langle q_{Nn_N}|p_{N-1n_{N-1}}\rangle \epsilon e^{-i(p_{N-1n_{N-1}}^2/2\mu)\Delta t} \cdots \langle p_{Nn_N}|q_{Nn_N}\rangle \epsilon e^{-iV(q_{Nn_N})\Delta t} \times \cdots$$
$$\langle q_{2n_2}|p_{1n_1}\rangle \epsilon e^{-i(p_{1n_1}^2/2\mu)\Delta t} \langle p_{1n_1}|q_{1n_1}\rangle \epsilon e^{-iV(q_{1n_1})\Delta t} \langle q_{1n_1}|\psi_i\rangle. \tag{77}$$

The next step is to "integrate" over the "momentum" variables. While this can be done exactly for quadratic functions of p in terms of Fresnel integrals, here this integral is replaced by a finite sum. The first step is to define a one time step free propagation operator. This is the q-space representation of the transfer matrix for free propagation [15][16] for a time Δt:

$$K(q'_m, q_n, \Delta t) dq_n := \sum_{l=-K}^{K} \langle q_m|p_l\rangle \epsilon e^{-i(p_l^2/2\mu)\Delta t} \langle p_l|q_n\rangle \epsilon =$$
$$\frac{\epsilon^2}{2\pi} \sum_{l=-K}^{K} e^{i(q'_m - q_n)p_l - i(p_l^2/2\mu)\Delta t}. \tag{78}$$

It follows from (68) that the integral over the initial coordinate is 1:

$$\int K(q', q, \Delta t) dq \to \sum_{n=-K}^{K} K(q_m, q_n, \Delta t)\epsilon = 1 \tag{79}$$

independent of q_m. Because of this, $K(q_m, q_n, \Delta t)dq$, is interpreted as the complex probability for making a transition from state q_n to state q_m in time step Δt. The probability interpretation follows because the sum is 1. In this case the sample set of probabilities is finite. The interpretation of equation (79) is that a state that ends up at q_m has to have started at one of the $2K+1$ q_n's with complex probability 1.

The path integral (77) can be expressed in terms of (79) as

$$\langle q_f|e^{-iHt}|q_i,\rangle \approx$$

$$\sum_{n_1\cdots n_N} K(q_f, q_{N,n_N}, \Delta t)e^{-iV(q_{N n_N})\Delta t}\epsilon K(q_{N,n_N}, q_{N-1,n_{N-1}}, \Delta t)e^{-iV(q_{N-1,n_{N-1}})\Delta t}\epsilon\cdots$$

$$\cdots K(q_{2,n_2}, q_{1,n_1}, \Delta t)e^{-iV(q_{1,n_1})\Delta t}\epsilon =$$

$$\sum_{n_1\cdots n_N} K(q_f, q_{N,n_N}, \Delta t)\epsilon K(q_{N,n_N}, q_{N-1,n_{N-1}}, \Delta t)\epsilon\cdots K(q_{2,n_2}, q_{1,n_1}, \Delta t)\epsilon\times$$

$$e^{-i\sum_{l=1}^{N} V(q_{l n_l})\Delta t}. \tag{80}$$

This is expressed as finite powers of products of finite-dimensional unitary transfer matrices.

Define

$$P_N(q_f, q_N, q_{N-1}, \cdots, q_2, q_1) :=$$

$$K(q_f, q_N, \Delta t)\epsilon K(q_N, q_{N-1}\Delta t)\epsilon\cdots K(q_3, q_2, \Delta t)\epsilon K(q_2, q_1, \Delta t)\epsilon \tag{81}$$

which represents free propagation from q_1 to q_f along a path through $q_2, q_3, \cdots q_N$. By (79) it follows that summing over all of q_{i,n_i} gives 1 independent of q_f,

$$\sum_{n_1,\cdots,n_N} P_N(q_f, q_N, q_{N-1}, \cdots, q_2, q_1) := 1 \tag{82}$$

It is now possible to define the space of paths between q_i and q_f. A path γ is a N-dimensional vector $(q_1, q_2, \cdots q_N)$ where each of the q_n can have one of the M discrete eigenvalues of q. This vector represents a path that starts at $q_1 = n_1\epsilon$ and after time Δt is at $q_2 = n_2\epsilon$, $\cdots$, and after $N-1$ time steps is at $q_N = n_N\epsilon$ and arrives at q_f after N time steps. The set of all M^N paths that end up at q_f is denoted by Γ.

The quantity $P_N(\gamma) := P_N(q_f; q_N, q_{N-1}, \cdots, q_2, q_1)$ is a complex number that is interpreted as the complex probability for a particle to travel on the path $\gamma = q_1 \to q_2 \to \cdots \to q_{N-1} \to q_N \to q_f$ since

$$\sum_{\gamma\in\Gamma} P_N(\gamma) = 1. \tag{83}$$

It is the discrete analog of the complex probability that path lies in a given cylinder set of paths.

For the path γ a potential "functional" of the path γ is defined by

$$W[\gamma] = e^{-i\sum_{n=1}^{N} V(q_n)\Delta t} \tag{84}$$

where the sum is over each of the $q_n \in \gamma$. With this notation the approximate transition amplitude is

$$\langle q_f, t_f | e^{-iHt} | q_i, t_i \rangle \approx$$

$$\sum_{n_1, n_2, \cdots, n_N = 1}^{M} P_N(q_f, q_{Nn_N}, q_{N-1n_{N_1}}, \cdots, q_{2n_2}, q_{1n_1}) \times e^{-i\sum_{k=1}^{N} V(\epsilon n_k)\Delta t} \delta_{q_{1n_1}, q_i} =$$

$$\sum_{\gamma \in \Gamma} P_N(\gamma) W[\gamma] \delta_{q_{1n_1}, q_i} \tag{85}$$

which is represented by the expectation $E[W\delta]$ of the potential functional $W[\gamma]\delta_{q_{1n_1}, q_i}$ with respect to the complex probability distribution $P_N(\gamma)$.

Note that this transition amplitude can be expressed exactly as the N-th power

$$X_{fj}^{N} \delta_{ji} \tag{86}$$

of the transfer matrix

$$X_{ij} := K_{ij} W_j \tag{87}$$

where

$$K_{ij} := K(q_j, q_k, \Delta t)\epsilon \qquad W_j := e^{-iV(q_j)\Delta t} \tag{88}$$

applied to the initial state. The important observation is that even though there are $(2K+1)^N$ discrete paths, the discrete path integral involves computing the N^{th} power of a single $(2K+1) \times (2K+1)$ dimensional matrix.

It is interesting to note that while the computation of the path integral is reduced to matrix multiplication, the matrix product can be deconstructed to find the contribution of each path to $E[W\delta]$.

In [12] a similar method was used to compute sharp momentum scattering transition matrix elements using real-time path integrals interpreted as expectation values of a potential functional with respect to a complex probability distribution on cylinder sets of paths. In that application the factorization of the complex probability into a product of one time step probabilities was only approximate and as a result unitarity was only satisfied approximately.

In [12] sharp momentum scattering matrix elements were approximated using a path integral approximation to matrix elements of the scattering transition operator

$$T_{fi} = \lim_{t \to -\infty} \langle k_f | V e^{-Ht} e^{-iH_0 t} | k_i \rangle. \tag{89}$$

The sharp momentum eigenstates $|k_{f/i}\rangle$ were replaced by normalizable states $|\Psi_I\rangle$ and $|\Psi_F\rangle$ that are sharply peaked about the initial and final momenta respectively and have spatial support in the interaction volume. They were normalized like delta functions in the sense that they integrate to 1.

In the form (89) the interaction V provides a convenient volume cutoff on the localized initial scattering state. The matrix $(K^\dagger)^N X^{2N} (K^\dagger)^N$, which converges to the scattering operator, is exactly unitary so it can be diagonalized with eigenvalues of the form $e^{2i\delta_n}$, where δ_n are eigenvalues of a phase shift operator.

The convergence of this method depends on the convergence of the Trotter limit and the convergence of the discrete quadrature. Mathematically the Trotter product formula converges strongly for suitable Hamiltonians; this was used in [11] to show that in the continuum case the expectation of the potential functional with respect to the complex probability associated with free propagation converges to global solutions of the Schrödinger equation. This suggests that final result is independent of the order of making the Trotter approximation and the discrete quadrature approximation.

This interpretation of the path integral as the expectation value of a random variable over a complex probability on a space of paths has a conceptual advantage over the conventional interpretation. In the conventional interpretation of the path integral in terms of the action functional, the finite difference representation of the "derivatives" in the action involves differences that never get small as the time steps get small, rendering the interpretation of the path integral as an integral over paths weighted by a "measure" depending on the action questionable. The representation in terms of complex probabilities involves a real potential functional defined on continuous paths. The potential functional can be thought of as a *perturbation of a complex Gaussian process* associated with free propagation.

VIII. 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

$$P_{fi} = |\langle\psi_f(t)|\psi_i(t)\rangle|^2. \tag{90}$$

While the individual states depend on time, the probability (90) is independent of t due to the unitarity of the time evolution operator. The important consideration is that both states have to be evaluated at the same time. The problem of scattering theory is that there is no common time when both the initial and final states are simple. On the other hand the initial state is simple before the collision and the final state is simple after the collision.

The initial and final states at the time of collision can be determined by evolving them from times where they behave like non-interacting subsystems to the collision time. Since localized wave packets spread, the effects of spreading can be eliminated by starting with localized wave packets at the collision time, evolving them beyond the range of interactions using free time evolution, and then evolving them back to the interaction region using the full Hamiltonian. The result is a unitary mapping that transforms the free wave packet at the collision time to the dynamical wave packet at the same time.

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

$$\||U(\pm\tau)|\psi_\pm(0)\rangle - U_0(\pm\tau)||\psi_{0\pm}(0)\rangle\| \approx 0 \tag{91}$$

where τ is sufficiently large for the interacting particles to be separated beyond the range of their mutual interactions. This expression is independent of τ for sufficiently large τ, but the minimum value of τ depends on the range of the interaction and the structure of $|\psi_{0\pm}(0)\rangle$. Normally dependence on these conditions is removed by taking the limit $\tau \to \infty$. In this work, for computational reasons, it is desirable to choose τ 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 (91) can be replaced by

$$\||\psi_{\pm}(0)\rangle - U(\mp\tau)U_0(\pm\tau)|\psi_{0\pm}(0)\rangle\| \approx 0. \tag{92}$$

The operators

$$\Omega_{\pm}(\tau) := U(\pm\tau)U_0(\mp\tau) \tag{93}$$

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

Using these definitions the scattering probability can be expressed as

$$P_{fi} = |\langle\psi_{0+}(0)|S(\tau)|\psi_{0-}(0)\rangle|^2 \tag{94}$$

where

$$S(\tau) := \Omega^{\dagger}(\tau)\Omega(-\tau) \tag{95}$$

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

$$S(\tau) = e^{2i\delta(\tau)} \tag{96}$$

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

In a real experimental measurement the probability (94) 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 [17] 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 is amenable to 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 [18][19][20].

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 the previous section

$$S(\tau) = \lim_{N\to\infty} K^{-N}X^{2N}K^{-N} \tag{97}$$

where

$$K_{ij} = K(q_i, q_j, \Delta t)\epsilon \qquad (X)_{ij} = K(q_i, q_j, \Delta t)\epsilon e^{-iV(q_j)\Delta t}, \tag{98}$$

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

$$K^N = K(f_f, q_i, N\Delta t). \tag{99}$$

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

$$S = I - 2\pi i\delta(E_f - E_i)T \tag{100}$$

where T is approximately given by

$$T_s \approx V\Omega(-\tau) \tag{101}$$

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

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

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

$$\langle q\rangle_\psi := \sum_{n=-K}^{K} \frac{\langle\psi|u_n\rangle n\epsilon\langle u_n|\psi\rangle}{\langle\psi|\psi\rangle} \qquad \langle p\rangle_\psi := \sum_{n=-K}^{K} \frac{\langle\psi|v_n\rangle n\epsilon\langle v_n|\psi\rangle}{\langle\psi|\psi\rangle} \tag{102}$$

$$(\Delta q)^2 = \langle\psi|(q - \langle q\rangle)^2|\psi\rangle = \sum_{n=-K}^{K} \frac{\langle\psi|u_n\rangle((n\epsilon)^2 - \langle q\rangle^2)\langle u_n|\psi\rangle}{\langle\psi|\psi\rangle} \tag{103}$$

$$(\Delta p)^2 = \langle\psi|(p - \langle p\rangle)^2|\psi\rangle = \sum_{n=-K}^{K} \frac{\langle\psi|v_n\rangle((n\epsilon)^2 - \langle p\rangle^2)\langle v_n|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{104}$$

The continuum delta function normalized minimal uncertainty states are

$$\langle p|\psi_0(0)\rangle = \frac{1}{2\sqrt{\pi}\Delta p} e^{-\frac{(p-\langle p\rangle)^2}{4(\Delta p)^2}}. \tag{105}$$

where $\langle p\rangle$ is the mean momentum and Δp 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 (105):

$$\langle p|\psi_0(-\tau)\rangle = \frac{1}{2\sqrt{\pi}\Delta p} e^{-\frac{(p-p_i)^2}{4(\Delta p)^2} + i\frac{p^2}{2\mu}\tau}. \tag{106}$$

In the discrete "p" representation this is replaced by

$$\langle n|\psi_0(-\tau)\rangle = Ce^{-\frac{(\epsilon n-\langle p\rangle)^2}{4(\Delta p)^2} + i\frac{n^2\epsilon^2}{2\mu}\tau}. \tag{107}$$

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

$$\langle m_q|\psi_0\rangle = \frac{\epsilon}{\sqrt{2\pi}} \sum_{n=-K}^{K} e^{i\epsilon^2 mn}\langle n|\psi_0(-\tau)\rangle. \tag{108}$$

To illustrate that this gives a good approximation to the continuum results $\langle p\rangle$, $\langle p\rangle$, Δq and Δp were calculated starting with $\langle p\rangle = 2.5$, $\Delta p = .25$ and $K = 300$ as input parameters in (106). The results of the calculation

$$\text{mean}_{p-calc} = 2.500000 \tag{109}$$

$$\text{mean}_{q-calc} = -2.51 \times 10^{-17} \tag{110}$$

$$\Delta_{p-calc} = .3000000 \tag{111}$$

$$\Delta_{q-calc} = 1.666667 \tag{112}$$

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

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

$$V(q) = \lambda e^{-\alpha q^2} \tag{113}$$

with $\lambda = .5$ and $\alpha = 2.0$. The potential is plotted in figure 1. The particle's mass is taken to be 1 in dimensionless units so the velocity and momentum can be identified. The initial wave packet is a Gaussian with a delta function normalization in momentum space with mean momentum $p = 2.5$ and width $\Delta p = .25$. It is pictured in figure 2. The Fourier transform of the initial wave packet is given in figure 3. The oscillations are due the to fact that 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 illustrates 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 [21].

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 [22] a Δp 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,τ and Δp that are needed for convergence. In practice there are a number of trade offs. Making the wave packets narrow in momentum increases the scattering volume in the coordinate representation. This in turn requires a larger τ to get out of the range of the potential. If τ gets too large the wave packet can move past $q_{max} = K\epsilon$ and will reappear at $q_{min} = -K\epsilon$. As p gets large the oscillations in the q space wave function have higher frequencies, which requires smaller time steps, while when p gets small it is necessary to make the wave packet width in momentum small enough so the coordinate space tail of the wave function gets out of the interaction volume.

The computations require storing the initial vector. It is not necessary to store the 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 q-bits can be used to represent large vectors.

This one-dimensional example approximated half-shell sharp-momentum transition ma-

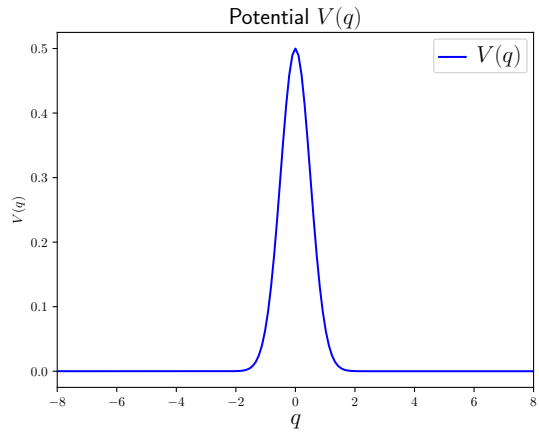

FIG. 1: **Potential**

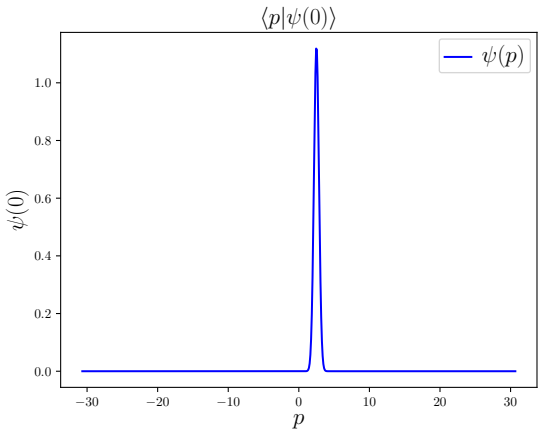

FIG. 2: **Momentum space initial Gaussian wave packet**

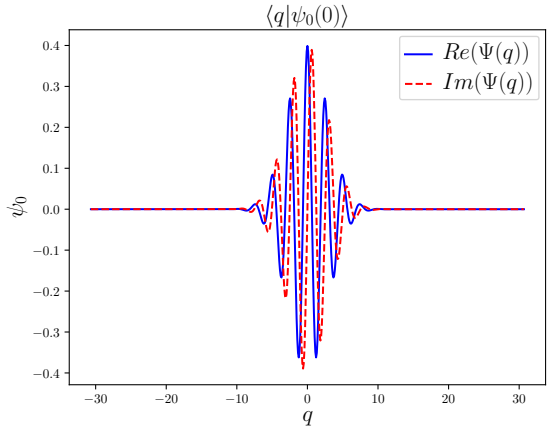

FIG. 3: **Coordinate space initial Gaussian wave packet**

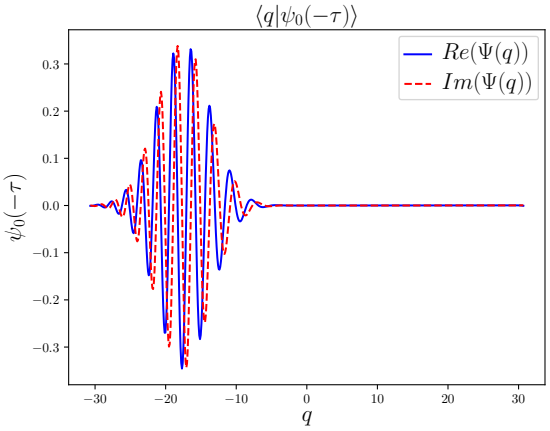

FIG. 4: **Free Gaussian wave packet at $\tau = -4$**

trix 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 operators has the advantage that the method can be formally extended to treat a large class of scattering problems.

The formulation of the discrete path integral used a reducible discrete Schwinger representation where the complex one time step probability is represented by a dense matrix. An equivalent irreducible representation in terms of qbits involves a product of matrices (40-41) that act on single qbits, which may have computational advantages.

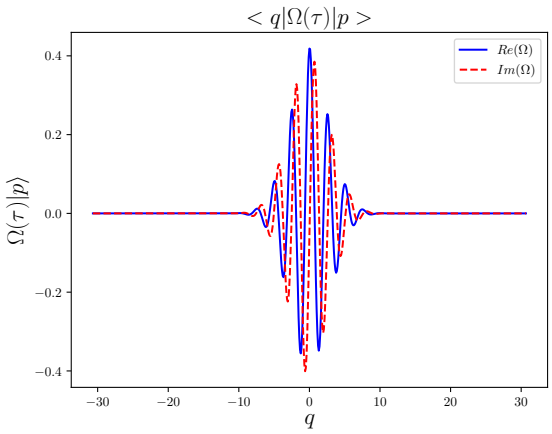

FIG. 5: **Initial scattering state at $t = 0$**

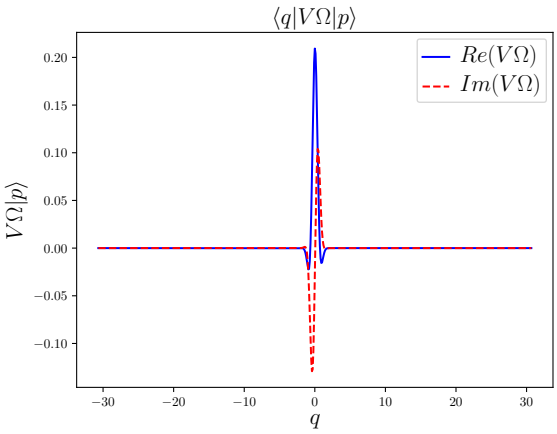

FIG. 6: **V $\times$ initial scattering state at $t = 0$**

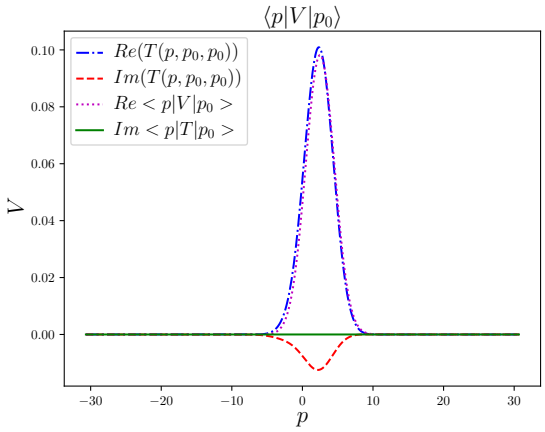

FIG. 7: $\langle p|V|\psi_{0i}(0)\rangle$

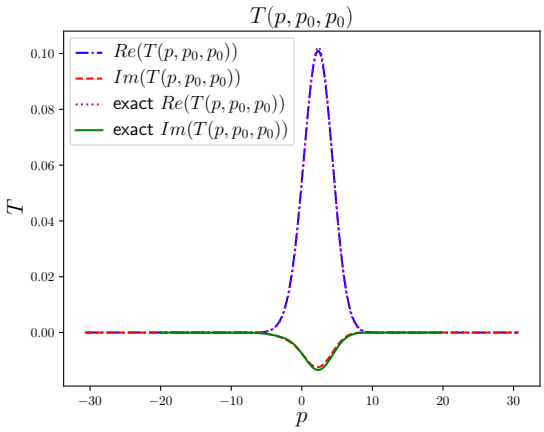

FIG. 8: $\langle p|T|\psi_{0i}(0)\rangle$

IX. 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 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.

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 are expected to be unimportant for the given reaction. Daubechies wavelets [23][24][25] and scaling functions are a basis for 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 for 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. Because they are complete they can be used to *exactly* expand canonical fields

$$\Phi(\mathbf{x},t) = \sum \Phi_n(t)\xi_n(\mathbf{x}) \qquad \Pi(\mathbf{x},t) = \sum \Pi_n(t)\xi_n(\mathbf{x}) \tag{114}$$

where $\Phi_n(t)$ and $\Pi_n(t)$ are discrete field operators. If the fields satisfy canonical equal time commutation relations

$$[\Phi(\mathbf{x},t),\Pi(\mathbf{y},t)] = i\delta(\mathbf{x}-\mathbf{y}) \tag{115}$$

then the discrete fields Φ_n and Π_n will satisfy discrete versions of the canonical equal time commutation relations [26] [27] [28]:

$$[\Phi_m(t),\Pi_n(t)] = i\delta_{mn} \qquad [\Phi_m(t),\Phi_n(t)] = 0 \qquad [\Pi_m(t),\Pi_n(t)] = 0. \tag{116}$$

In terms of these degrees of freedom the Hamiltonian for a ϕ^4 theory has the form

$$H = \frac{1}{2}\sum_n \Pi_n\Pi_n + \frac{m^2}{2}\sum_n \Phi_n\Phi_n + \sum_{mn} D_{mn}\Phi_m\Phi_n + \lambda\sum_{klmn}\Gamma_{klmn}\Phi_k\Phi_l\Phi_m\Phi_n \tag{117}$$

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

$$D_{mn} = \frac{1}{2}\int \boldsymbol{\nabla}\xi_n(\mathbf{x})\cdot\boldsymbol{\nabla}\xi_m(\mathbf{x})d\mathbf{x} \tag{118}$$

$$\Gamma_{klmn} = \int \xi_k(\mathbf{x})\xi_l(\mathbf{x})\xi_m(\mathbf{x})\xi_n(\mathbf{x})d\mathbf{x}. \tag{119}$$

For the wavelet basis these constants vanish unless all of the functions appearing in the integrals have a common support, which makes them almost local. In addition, because all of the functions in the integrand are related by translations and scale transformations to a single function, the integrals can all be expressed as linear combinations of solutions of some small linear systems generated by the renormalization group equation (120). Unlike a lattice truncation, the wavelet representation of the field theory is (formally) exact (before truncation). The basis functions regularize the fields so local products of fields that appear in the Hamiltonian are replaced by infinite sums of well-defined products of discrete field operators. The basis functions are differentiable, so there are no finite difference approximations.

Wavelet representations of quantum field theories have been discussed by a number of authors [29] [30] [31] [32] [33] [34] [35] [36] [37] [38] [38] [39] [26] [40] [41] [42] [43] [44] [45] [46] [27] [47] [48] [28] [49].

What is relevant is that the Hamiltonian (117) has the same form as (72), 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 Φ_n operators. Because all of the basis functions are constructed from the fixed point $s(x)$ of the renormalization group equation (120) the constant quantities D_{mn} and Γ_{klmn} can be expressed in terms of a finite set of elementary integrals.

The advantage of this basis is that it has natural volume and resolution truncations. For reactions taking place in a finite volume with a finite energy a (large) finite number of these degrees of freedom should provide a good approximation. This reduces the problem to a problem with a finite number of discrete degrees of freedom. In addition the truncated Hamiltonian still has the form (117), 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 VIII. For a quantum field theory the vector representing the state of the field will be much larger than in the one degree of freedom scattering case.

The construction of the wavelet basis used to construct the discrete representation of the Hamiltonian (117) is outlined below. The starting point the solution of the linear

renormalization group equation

$$\boxed{s(x) = \sum_{l=0}^{2L-1} h_l DT^l s(x)} \tag{120}$$

where

$$Df(x) := \sqrt{2} f(2x) \qquad \text{and} \qquad Tf(x) := f(x-1) \tag{121}$$

are unitary discrete dyadic scale transformations and unit translations. The h_l are constants that depend on the choice of L. Generally as L increases the solutions, $s(x)$, become smoother but the support increases. A useful case is $L = 3$ where the solution $s(x)$ of (120), called the scaling function, has support on $[0, 2L-1] = [0, 5]$ and has one continuous derivative. In that case the coefficients h_l for the Daubechies $L = 3$ scaling functions are

$$\begin{aligned}
h_0 &= (1 + \sqrt{10} + \sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\
h_1 &= (5 + \sqrt{10} + 3\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\
h_2 &= (10 - 2\sqrt{10} + 2\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\
h_3 &= (10 - 2\sqrt{10} - 2\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\
h_4 &= (5 + \sqrt{10} - 3\sqrt{5 + 2\sqrt{10}})/16\sqrt{2} \\
h_5 &= (1 + \sqrt{10} - \sqrt{5 + 2\sqrt{10}})/16\sqrt{2}.
\end{aligned} \tag{122}$$

They are chosen so the solution of (120) and unit translates are orthonormal and locally finite linear combinations of these unit translates can be used to locally pointwise represent degree 2 polynomials. Given the solution, $s(x)$, of (120) new functions are constructed from $s(x)$ by rescaling and translating

$$s_n^k(x) := D^k T^n(x) s(x) = \sqrt{2^k} s(2^k x - n). \tag{123}$$

The starting scale is fixed using

$$\int s(x) dx = 1. \tag{124}$$

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

$$\mathcal{S}^k := \{f(x) | f(x) = \sum_{n=-\infty}^{\infty} c_n s_n^k(x) \qquad \sum_{n=-\infty}^{\infty} |c_n|^2 < \infty\}. \tag{125}$$

The renormalization group equation (120) implies

$$\mathcal{S}^k \subset \mathcal{S}^{k+1}. \tag{126}$$

It follows that

$$\mathcal{S}^{k+1} = \mathcal{S}^k \oplus \mathcal{W}^k. \tag{127}$$

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

$$w_n^k(x) = D^k T^n w(x) \tag{128}$$

where

$$w(x) := \sum_{l=0}^{2L-1} (-)^l h_{2L-1-l} D T^l s(x) \tag{129}$$

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

$$\boxed{L^2(\mathbb{R}) = \mathcal{S}^k \oplus_{l=0}^{\infty} \mathcal{W}^{k+l}.} \tag{130}$$

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

$$\{\xi_n(x)\}_{n=-\infty}^{\infty} := \{s_n^k(x)\}_{n=-\infty}^{\infty} \cup \{w_n^m(x)\}_{n=-\infty, l=k}^{\infty}. \tag{131}$$

For the choice $L = 3$ the basis functions $s_n^k(x)$ and $w_n^k(x)$ have compact support on $[2^{-k}n, 2^{-k}(n+5)]$. All of the basis functions have one continuous derivative so the coefficients (118) are defined . The functions $s_n^k(x)$ are like splines in that linear combinations can be used to locally pointwise represent degree 2 polynomials while the functions $w_n^l(x)$ are orthogonal to the same polynomials on their support. The Fourier transforms of the basis functions are entire functions due to their compact support. Orthonormal three dimensional basis functions are products of one-dimensional basis functions. In spite of these nice properties, the basis functions are fractal valued (since they are related to fixed points of a renormalization group equation) and cannot be written down in closed form.

In order to use this representation the constant coefficients D_{mn} and $\Gamma_{n_1 \cdots n_k}$ that appear in the Hamiltonian (117) need to be computed. Using scale transformations (121) and the renormalization group equation (120) they can all be expressed in terms of the integrals

$$d_n = \int \frac{ds(x)}{dx} \frac{ds(x-n)}{dx} dx \qquad -4 \leq n \leq 4 \tag{132}$$

$$\gamma_{m,n,k} = \int s(x)s(x-m)s(x-n)s(x-k)dx \qquad -4 \leq mnk \leq 4. \tag{133}$$

These integrals are related to each other by finite linear equations derived from the renormalization group equation (120) and the scale fixing condition (124). These linear systems can formally be solved in terms of the coefficients h_l (122). The coefficients d_n are rational numbers and can be found in the literature on wavelets [50]. To find the γ_{mnk} requires finding eigenvalues of a $9^3 \times 9^3$ matrix. This eliminates the need be able to evaluate fractal valued functions. Alternatively the integrals γ_{mnk} can be approximated by noting that the renormalization group equation (120) and the scale fixing condition (124) can be used to exactly calculate the basis functions and their derivatives exactly at all dyadic rational points. Since the functions and their derivatives are continuous this can be used to estimate these quantities and integrals involving these quantities to any desired accuracy.

In order to illustrate a path integral treatment of this system consider a truncation of the theory in 1+1 dimension where only 2 adjacent modes of the Hamiltonian (117) are retained. In this case the overlap coefficients that appear in the Hamiltonian and couple adjacent modes can be expressed in terms of the following quantities

$$\Gamma_{0000} = 0.9528539 \tag{134}$$

$$\Gamma_{0001} = 0.0670946 \tag{135}$$

$$\Gamma_{0011} = 0.0890895 \tag{136}$$

$$\Gamma_{0111} = -0.1424536 \tag{137}$$

$$D_{00} = 295./56.; \tag{138}$$

$$D_{01} = -356./105.; \tag{139}$$

$$D_{10} = D_{01}; \tag{140}$$

$$D_{11} = D_{00} \tag{141}$$

where the Γ 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

$$H = \frac{1}{2}\sum_{n=0}^{1} \Pi_n \Pi_n + \frac{m^2}{2}\sum_{n=0}^{1} \Phi_n \Phi_n + \sum_{mn} D_{mn}\Phi_m\Phi_n + \lambda \sum_{klmn=0}^{1} \Gamma_{klmn}\Phi_k\Phi_l\Phi_m\Phi_n \tag{142}$$

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.

$$H \to H_F \tag{143}$$

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 calculation 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.

$$U_F(\tau) = e^{-iH_F\tau} = \lim_{N\to\infty}(e^{-iH_F(\Pi)\Delta t}e^{-iH_F(\Phi)\Delta t})^N \tag{144}$$

where $\Delta t = \tau/N$ and

$$H_F = H_F(\Pi) + H_F(\Phi) \tag{145}$$

with

$$H_F(\Pi) := \frac{1}{2}\sum_n \Pi_n\Pi_n \tag{146}$$

and

$$2H_F(\Phi) := \frac{m^2}{2}\sum_n \Phi_n\Phi_n + \sum_{mn} D_{mn}\Phi_m\Phi_n + \lambda\sum_{klmn}\Gamma_{klmn}\Phi_k\Phi_l\Phi_m\Phi_n \tag{147}$$

which expresses H_F as the sum of a part with only the Π_n fields and another part with only the Φ_n fields. Since the discrete canonical pairs of field operators Φ_n and Π_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 Φ_n and Π_n by a collection of $M = 2K + 1$ closely spaced eigenvalues $\phi_n, \pi_n = n\epsilon$ where $-K \leq n \leq K$ and $\epsilon^2 = 2\pi/M$. This is exactly what was done in the one-dimensional case, 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 $\langle \boldsymbol{\phi}|\chi\rangle = \chi(n_1\epsilon, \cdots, n_F\epsilon)$ 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 path integrals to calculate the time evolution of these coupled modes. For the field theory, before truncation, in the discrete representation there are integrals over an infinite number of modes. For the discarded modes the volume being integrated over for each mode is infinite, resulting in an infinite product of an infinite number of infinite irrelevant constants. The advantage of discretizing the integrals is that the volume for each mode is finite:

$$\text{Volume} = \sqrt{2M\pi} - \sqrt{2\pi/M}.$$

The discarded modes can be eliminated by summing and dividing by this finite volume, mode by mode, before taking the continuum limit. In this way the integrals over discarded degrees of freedom are replaced by a product of 1's. This results in a path integral that only involves the retained degrees of freedom. The discrete approximation results in a sample space with a finite number of discrete paths.

The Trotter approximation is

$$\langle n_1, n_2, \cdots n_F|U_F(\tau)|\chi(0)\rangle =$$

$$\lim_{N\to\infty} \langle n_1, n_2, \cdots n_F|(e^{-iH_f(\Pi)\Delta t}e^{-iH_F(\Phi)\Delta t})^N|\chi(0)\rangle. \tag{148}$$

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:

$$\int d\boldsymbol{\phi} = \epsilon^F \sum_{n_1=-K}^{K} \cdots \sum_{n_F=-K}^{K}, \tag{149}$$

for vectors representing a value of the eigenvalues of each of the F independent ϕ fields,

$$\boldsymbol{\phi} = (n_1\epsilon, \cdots, n_F\epsilon) \qquad -K \leq n_i \leq K, \tag{150}$$

for vectors representing the value of the eigenvalues of each of the F independent π fields

$$\boldsymbol{\pi} = (n_1\epsilon, \cdots, n_F\epsilon) \qquad -K \leq n_i \leq K \tag{151}$$

and

$$\gamma = (\boldsymbol{\phi}_0, \boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_N) \tag{152}$$

for a "path" that ends at $\boldsymbol{\phi}_0$ where $\boldsymbol{\phi}_j$ $(j > 0)$ represents values of each of the ϕ_n fields at each of N time steps.

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

$$K(\boldsymbol{\phi}', \boldsymbol{\phi}, \Delta t) := \sum_{\mathbf{n}''} \langle \boldsymbol{\phi}' | \boldsymbol{\pi} \rangle \Delta t \langle \boldsymbol{\pi} | \boldsymbol{\phi} \rangle. \tag{153}$$

It follows from (68) that $K(\boldsymbol{\phi}', \boldsymbol{\phi}, \Delta t)$ has the property

$$\sum_{\mathbf{n}} K(\boldsymbol{\phi}', \boldsymbol{\phi}, \Delta t)\epsilon^F = 1 \tag{154}$$

and

$$P(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \cdots \boldsymbol{\phi}_1) :=$$

$$K(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \Delta t)\epsilon^F K(\boldsymbol{\phi}_N, \boldsymbol{\phi}_{N-1}, \Delta t)\epsilon^F \cdots K(\boldsymbol{\phi}_3, \boldsymbol{\phi}_2, \Delta t)\epsilon^F K(\boldsymbol{\phi}_2, \boldsymbol{\phi}_1, \Delta t)\epsilon^F \tag{155}$$

also satisfies

$$\sum_{\gamma \in \Gamma} P(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \cdots, \boldsymbol{\phi}_1) = 1. \tag{156}$$

Equation (155) represents the complex probability of a given path, where at each time slice each of the F ϕ's has one of M allowed values between $-K\epsilon$ and $K\epsilon$. Removing the last factor of ϵ^F and only summing over $\boldsymbol{\phi}_N \cdots \boldsymbol{\phi}_2$ gives the evolution due to free propagation

$$\langle \boldsymbol{\phi}_f | e^{-\frac{i}{2}\boldsymbol{\Pi}\cdot\boldsymbol{\Pi}\tau} | \boldsymbol{\phi}_1 \rangle = \sum_{\boldsymbol{n}_n \cdots \boldsymbol{n}_1} P(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \cdots, \boldsymbol{\phi}_1)\epsilon^{-F}. \tag{157}$$

The full path integral including the effects of the interaction can be expressed as the expectation of the following potential functional of the path γ with respect to the complex probability distribution (85):

$$W[\gamma] := e^{i\sum_n H_F(\boldsymbol{\phi}_n)\Delta t} \tag{158}$$

where $H_F(\boldsymbol{\phi}_n)$ represents the value of the ϕ-dependent part of the Hamiltonian evaluated at the value of the path γ at the n-th time slice.

This gives the path integral approximation

$$\langle n_{1f}, n_{2f}, \cdots n_{Ff}|U_F(\tau)|\chi(0)\rangle =$$

$$\sum_{\gamma} P(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \cdots \boldsymbol{\phi}_1) W[\gamma]\chi(\boldsymbol{\phi}_1) \tag{159}$$

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

$$P(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \cdots \boldsymbol{\phi}_1) W[\gamma] =$$

$$K(\boldsymbol{\phi}_f, \boldsymbol{\phi}_N, \Delta t) e^{iH_F(\boldsymbol{\phi}_N)\Delta t}\epsilon^F K(\boldsymbol{\phi}_N, \boldsymbol{\phi}_{N-1}, \Delta t) e^{iH_F(\boldsymbol{\phi}_{N-1})\Delta t}\epsilon^F \cdots$$

$$K(\boldsymbol{\phi}_3, \boldsymbol{\phi}_2, \Delta t) e^{iH_F(\boldsymbol{\phi}_2)\Delta t}\epsilon^F K(\boldsymbol{\phi}2, \boldsymbol{\phi}_1, \Delta t) e^{iH_F(\boldsymbol{\phi}_1)\Delta t}\epsilon^F. \tag{160}$$

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

At each stage these calculations use finite mathematics. The use of the finite Weyl representation exactly preserves unitary at each level of approximation. Both the $\boldsymbol{\phi}$ and $\boldsymbol{\pi}$ 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.

The calculation shown in figures nine and ten show 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

$$\langle \phi_1, \phi_2|\psi\rangle = Ne^{-\sum_{i=0}^{1}(\phi_i - \langle\phi_i\rangle)^2/(4\delta\phi_i^2)} \tag{161}$$

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

Figures 13 and 14 show plots of the real and imaginary parts of ϕ_0 when $\phi_1 = 0$ 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.

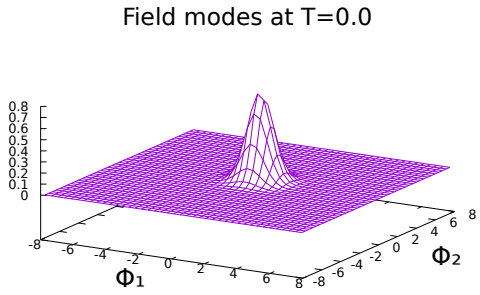

FIG. 9: **Two modes (real) at T=0**

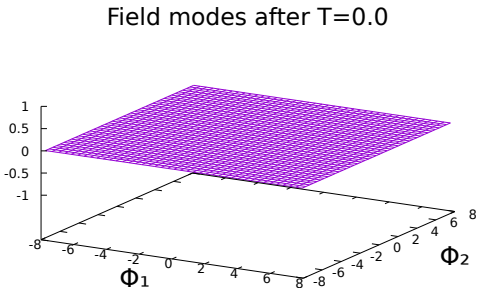

FIG. 10: **Two modes (imaginary) at T=0**

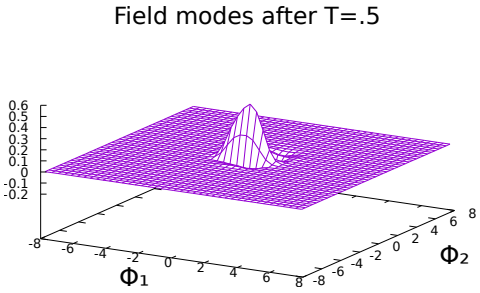

FIG. 11: **Two modes (real) after T=.5**

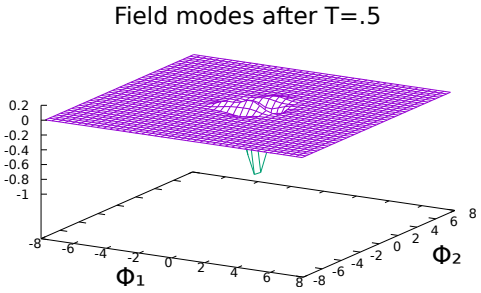

FIG. 12: **Two modes (imaginary) after T=.5**

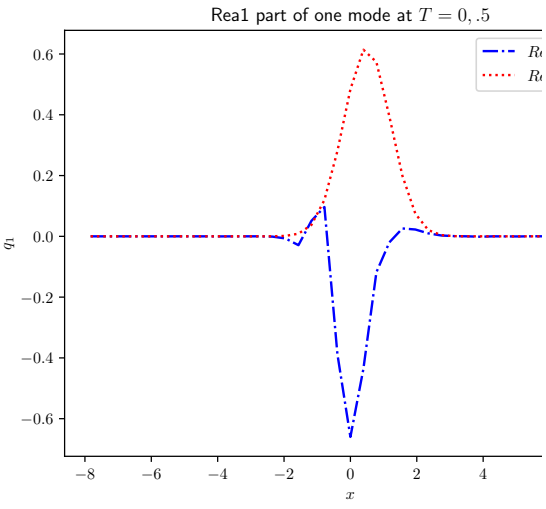

FIG. 13: **One mode (real) after T=0.,.5**

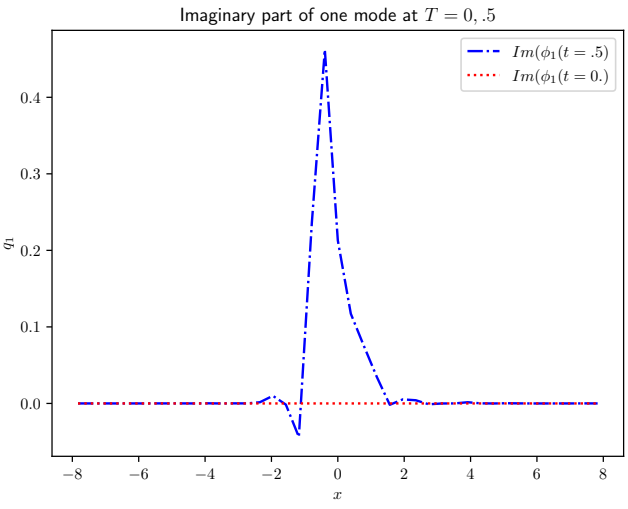

FIG. 14: **One mode (imaginary) after T=0.,.5**

X. SUMMARY AND CONCLUSION

This paper discusses a path integral treatment of discrete representations of quantum theory. The treatment is motivated by a textbook treatment [1] of measurement theory of quantum systems on finite dimensional Hilbert spaces. The discrete representation provides a natural connection to a q-bit representation in terms of an irreducible set of quantum gates. It was also shown to formally provide a discrete path integral treatment of problems in potential scattering and quantum field theory. The discrete Weyl representation is closely related to the quantum Fourier transform while the equivalent decomposition into irreducible sub algebras is more directly related to quantum circuits.

The treatment starts by considering a general quantum observable with a finite number of outcomes. It is used to construct a pair of unitary operators, one that commutes with the original observable and a second complementary unitary operator. The two unitary operators are a finite dimensional version of the irreducible Weyl algebra on the Hilbert space spanned by the eigenvectors of the original operator. When the dimension of the Hilbert space gets large this algebra approximates the Weyl algebra of a continuum theory. When the large number is a power of 2 the algebra can be decomposed into a product of irreducible sub-algebras where the complementary unitary operators are elementary qbit gates, which are the building blocks of quantum circuits.

In the limit of large dimensions discrete operators that behave like canonical coordinates and momenta can be constructed from this algebra. In this approximation the "coordinates" and "momenta" take on a finite number of discrete values that get closer together and cover more of the real line as the number of degrees of freedom increases.

Hamiltonians that are sums of an operator that is quadratic in the "momentum" variables and an operator that is a multiplication operator in the "coordinate" variables are considered. Time evolution is represented by a product of transfer matrices for a large number of small steps. For small time steps the transfer matrix can be approximately factored into a product of a transfer matrix involving the "momentum" part of the Hamiltonian and another transfer matrix involving the "coordinate" part of the Hamiltonian. Both of these transfer matrices are represented in the discrete "coordinate" representation. A path is defined to go through one of the discrete coordinates at each time step. In the discrete representation the number of possible paths is M^N where N is the number of time steps and M is the number of discrete

coordinates at each time slice.

The transfer matrices involving the momentum part of the Hamiltonian have the property that summing over either the initial or final coordinates gives 1, independent of the other coordinate. In this work the momentum transfer matrix is interpreted as the complex probability for a transformation from one of the allowed coordinates to another one in time step Δt. The product of N of these operators, where the final coordinate of one is the initial coordinate of the next one is interpreted as a complex probability for a given "path" on the finite sample set of discrete paths. This probability has the property that summing over all paths with a given starting point or a given end point is 1. The interaction (coordinate dependence) is included by multiplying this probability by the product of the coordinate transfer matrices evaluated at each point on the path. In this interpretation the coordinate contribution is represented by a functional on the space of paths. Taking the expectation value of this functional with respect to the complex probability distribution gives the usual Trotter product representation of finite time evolution of the discrete system.

In the discrete representation all of the operators are exactly unitary and the mathematics is finite. The sample space of paths for the complex probabilities is finite. The general structure of the Hamiltonian as the sum of a quadratic form in the momentum variables and an interaction term is realized in non-relativistic quantum mechanics and relativistic quantum field theory. The application to potential scattering was discussed using the example of a particle scattering from a smooth short range interaction in one dimension. In the case of field theories an exact multi-resolution representation of the field in terms of an infinite number of discrete modes was used. When truncated to a finite number of modes the resulting discrete system has the structure of system of coupled particles.

The long term interest is in quantum computing. The examples were computed by applying products of the one step transfer matrices to an initial vector. By computing the transfer matrix elements on the fly, is was not necessary to store the transfer matrix. However as the number of degrees of freedom is increased, the size of the vector representing the state of the quantum system is the major limitation.

The author would like to thank William Hester for pointing out some errors in the original

version of this manuscript.

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