Simulation of many-body interactions by conditional geometric phases

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It is shown how to exactly simulate many-body interactions and multi-qubit gates by coupling finite dimensional systems, e.g., qubits with a continuous variable. Cyclic evolution in the phase space of such a variable gives rise to a geometric phase, depending on a product of commuting operators. The latter allows to simulate many-body Hamiltonians and nonlinear Hamiltonians, and to implement a big variety of multi-qubit quantum gates on both qubits and encoded qubits. An application to the quantum amplitude amplification algorithm will be discussed.

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I. INTRODUCTION

One of the most challenging and interesting problems in theoretical physics concerns the understanding of quantum many-body systems. In view of the exponentially many degrees of freedom involved, it is generally agreed that simulation of such systems is a task that cannot be efficiently tackled by any classical computers. On the other hand, as suggested by Feynman [4] the growth in computational resources is only linear on a quantum computer [6], which is itself a quantum many-body system. Therefore even a modest size quantum computer, e.g., containing only a few tens of qubits, could outperform a classical computer. We should like to stress that the feasibility of such a “devoted” quantum computer problem is expected to be definitely greater than the one of a general purpose quantum computer [13].

Simulation of Hamiltonians has very practical applications in quantum control [4] and quantum information theory [8]. A typical goal is to achieve, i.e., simulate, as many as possible desired entangling Hamiltonians starting from a given one and the ability to perform local operations [9,10] or more generally to enact transformations drawn from a given “natural” set of available interactions.

If we have two Hamiltonians \(H_1\) and \(H_2\) we can simulate the Hamiltonian \(\lambda_1 H_1 + \lambda_2 H_2\) (\(\lambda_1\) and \(\lambda_2\) are real numbers) and the Hamiltonian \(i[H_1,H_2]\) [1]. Thus any Hamiltonians in the algebra generated by \(H_1\) and \(H_2\) can be simulated. This simulation method does not require that the two Hamiltonians \(H_1\) and \(H_2\) commute but require that one can alternately turn on them for arbitrarily short time over infinite steps. Physically switching Hamiltonians over arbitrarily short time is not an easy task and unrealistic in some sense. We shall propose a method to do exact Hamiltonian simulations over finite steps.

In this paper we consider a “hybrid” physical system consisting of \(N\) qubits coupled with a continuous variable system. The state space is then given by \(\mathcal{H} = (\mathcal{F}^2)^\otimes N \otimes h_\infty\), where \(h_\infty := \text{span}\{|n\rangle\}_{n=0}^\infty\) is the standard Fock space for a single mode described by the bosonic annihilation and creation operators \(a\) and \(a^\dagger\), respectively. We assume the following Hamiltonians [12,13]

\[
H_1 = -i\lambda(aa^\dagger - a^\dagger a) \hat{A}, \tag{1}
\]

\[
H_2 = \omega a^\dagger a \hat{A}, \tag{2}
\]

The operator \(\hat{A}\) is a pure qubit operator that in the sequel will be mostly either a Pauli operator \(\sigma_{\alpha}(\alpha = x,y,z)\) for ion \(i\) or a collective angular momentum operator \(J_\alpha = \frac{1}{2} \sum_{i=1}^N \sigma_{\alpha i}\). The case of \(\hat{A} = J_\alpha\) corresponds to \(N\) ions with each driven by identical Raman lasers. From the Hamiltonians above we can have the conditional displacement operator and the conditional rotation operator

\[
U_1 = e^{-iH_1t} = e^{-i\lambda \hat{A}(a^\dagger a - a a^\dagger)} , \tag{3}
\]

\[
U_2 = e^{-iH_2t} = e^{-i\omega t \hat{A} a^\dagger a} , \tag{4}
\]

respectively. These two operators will play a crucial role in this paper in which we will try to address the following question: given these two kinds of physical operators, what is the maximal set of Hamiltonians that we can simulate? In Ref. [14] it has been shown that a conditional displacement of the vibrational mode of trapped ions can be used to simulate nonlinear collective and interacting spin systems including nonlinear tops and a universal two–qubit gate, independent of the vibrational state of the ion. The scheme in [14] has been further extended in order to realize the nonlinear Hamiltonian \(J_\alpha^2\) [13] and multi-qubit quantum gates [10].

A general framework for quantum information processing (QIP) with hybrid quantum systems has been proposed in Ref. [15]. There it has been proved that an universal set of Hamiltonians for hybrid quantum computation is provided by the following: \(\{\pm\sigma_x \hat{x}, \pm \sigma_z \hat{x}, \pm \sigma_z \hat{p}\}\). The position and momentum operators \(\hat{x}\) and \(\hat{p}\) satisfy the canonical commutation relation \([\hat{x}, \hat{p}] = i\). The ability to turn on and off the Hamiltonians from this set allows one to produce conditional displacements that in turns allow to enact Hamiltonians that are arbitrary polynomials of the \(\sigma_x, \sigma_y, \sigma_z, \hat{x}\), and \(\hat{p}\). We can use an alternative set of Hamiltonians \(\{\sigma_x a^\dagger a, \sigma_z a^\dagger a, \hat{x}\}\). This set can be easily reduced to the above one as follows:
If $\alpha x \in \alpha x$ is the state $|0\rangle$ or $|1\rangle$. These equations show that not only conditional displacements but also conditional rotations are useful in quantum computers. We will use both the conditional displacement operators and conditional rotation operators to simulate many-body interactions in quantum optical systems. The operator $\hat{D}$ is given by [12]. Phase-space translations are represented by the displacement operator $\hat{D}_{\alpha}$ and algorithms [14,20].

Our scheme is interestingly related to one kind of geometric phase, i.e., the geometric phase in phase space [21,22]. However now our geometric phase is dependent on some operators, i.e., it is a conditional geometric phase. Recently both the adiabatic [23] and non-adiabatic [24] geometric phases have been suggested as potential candidates for realizing quantum computers displaying some built-in fault tolerant features [25–29].

We shall see that even geometric phases in phase space could be useful for QIP.

1. GEOMETRIC PHASES IN PHASE SPACE

We begin by a brief review of the geometric phase within the formalism recently given by Liu [22]. Phase-space translations are represented by the displacement operator

$$D(\alpha) \equiv D(\sqrt{2}a) = e^{i(\alpha x + \beta)} \hat{p}.$$

where the complex quantity $\alpha = x + ip$ parametrizes the displacement and $D(\alpha) = \exp(\alpha a^\dagger - \alpha^* a)$ is the usual displacement operator in quantum optics. These operators satisfy the relation

$$D(\beta)D(\alpha) = e^{i \text{Im} (\beta^* \alpha)} D(\alpha + \beta).$$

From Eq. (9) it follows also the useful identity

$$e^{i \text{Im} (\beta^* \alpha)} = D(-\beta)D(-\alpha)D(\beta)D(\alpha).$$

We consider now a closed loop $\gamma$ which is an $N$-sided polygon with sides $\alpha_j$ ($j = 1, 2, ..., N$) such that $\sum_{j=1}^{N} \alpha_j = 0$. The total transformation associated with $\gamma$ is given by [22]

$$D_{\gamma} = D(\alpha_N) \cdots D(\alpha_1).$$

An arbitrary closed loop $\gamma$ can be approached in the limit of $N \to \infty$. In this case the total transformation is just a phase factor $D_{\gamma} = \exp(\text{i} \Theta)$, where

$$\Theta = \frac{1}{2} \oint (x dp - \beta dx).$$

The phase $\Theta$ neither depends on the form of the loop nor on the speed of the transformation but just on the area of the loop. For this reason it deserves the name of a geometric phase.

2. SIMULATION OF MANY-BODY INTERACTIONS

Let us recall the Hamiltonian simulation [9]. There is a set of Hamiltonians $\{H_i\}$ and a class of allowed operations like local unitaries or local operations and classical communications. The aim is to produce a desired evolution $e^{-iHt}$ from the set of the Hamiltonians and the class of allowed operations, where $H$ is the simulated Hamiltonian the $t$ is the simulated time.

Sometimes the class of local operations is not cheap resource. In this paper we will not use them and just begin from a set of Hamiltonians to do the simulation.

A. Nonlinear Hamiltonians and two-body interactions

A conditional displacement operator reads $D(\hat{A} \alpha)$, where the Hermitian operator $\hat{A}$ usually represents a discrete variable observable. By using the spectrum decomposition of the operator $\hat{A}$, $\hat{A} = \sum_{k=1}^{N} \lambda_k |k\rangle \langle k|$ the displacement operator can be written as

$$D(\hat{A} \alpha) = \sum_{k=1}^{N} |k\rangle \langle k| D(\lambda_k \alpha).$$

From the above equation one can see clearly that the amount of displacement is dependent on the eigenvalues of $\hat{A}$. By replacing the displacement operators in Eq. (10) with conditional displacement operators, we immediately obtain
\[ e^{i\theta \hat{A}\hat{B}} = \mathcal{D}( -\hat{B}\beta ) \mathcal{D}( -\hat{A}\alpha ) \mathcal{D}( \hat{B}\beta ) \mathcal{D}( \hat{A}\alpha ), \]  \hfill (14) 

where \( \theta = \text{Im}(\beta^*) \) and operator \( \hat{B} \) commutes with \( \hat{A} \). Now the geometric phase depends on the operator product \( \hat{A}\hat{B} \). Therefore we can simulate the Hamiltonian \( \hat{A}\hat{B} \) if operators \( \hat{A} \) and \( \hat{B} \) commute and belong to one system. For example if \( \hat{A} = \hat{B} = J_z \), we get the nonlinear Hamiltonian \( J_z^2 \), which is useful for creating GHZ multipartite entangled states \([32]\) and generate spin–squeezed states \([32]\). If \( \hat{A} \) and \( \hat{B} \) belong to different systems we may simulate the two–body interaction Hamiltonian \( \hat{A}\hat{B} \).

**B. Three–body interactions**

In the context of NMR quantum computation, Tseng et al. \([22]\) proposed a method to simulate three–body interaction of the type \( \sigma_z \otimes \sigma_z \otimes \sigma_z \). Due to the self–inverse property of \( \sigma_z \) simulation of the three–body Hamiltonian becomes relatively easy by two–body interactions. The simulation can be obtained in the following way

\[ e^{-i\theta \sigma_x \otimes \sigma_x \otimes \sigma_x} = e^{-i\hat{\sigma}_x \sigma_x \otimes \sigma_x \otimes \sigma_x} e^{i\theta \sigma_x} = e^{i\hat{\sigma}_x \sigma_x \otimes \sigma_x \otimes \sigma_x} e^{i\theta \sigma_x}, \]  \hfill (15) 

Now we show how to create ‘nonphysical’ three–body interaction Hamiltonians \( H = \hat{A}\otimes \hat{B}\otimes \hat{C} \) for general operators \( \hat{A}, \hat{B}, \) and \( \hat{C} \) which act on three different subsystems, respectively. To this aim let us introduce the operator \( R(\theta) = \exp( i\theta a I ) \), it entails a rotation in the phase space

\[ R(-\theta) \begin{pmatrix} \hat{x} \\ \hat{p} \end{pmatrix} R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{p} \end{pmatrix}. \]  \hfill (16) 

Directly from the above equation we obtain

\[ \mathcal{D}( a e^{i\theta} ) = R(\theta) \mathcal{D}( a ) R(-\theta). \]  \hfill (17) 

The conditional rotation operator is given by \( R(\theta \hat{C}) \), which makes a rotation in phase space conditioned on the operator \( \hat{C} \). As in Eq.(17) we get

\[ \mathcal{D}( a e^{i\theta \hat{C}} ) = R(\theta \hat{C}) \mathcal{D}( a ) R(-\theta \hat{C}). \]  \hfill (18) 

Then we can replace \( a \) with \( a e^{i\theta \hat{C}} \) in Eq.(14) and obtain

\[ e^{-i\tau \hat{A}\otimes \hat{B}\otimes \sin(\theta \hat{C} + \phi)} = \mathcal{D}( -\hat{B}\beta ) \mathcal{D}( -\hat{A} e^{i\theta \hat{C}} ) \mathcal{D}( \hat{B}\beta ) \mathcal{D}( \hat{A} e^{i\theta \hat{C}} ), \]  \hfill (19) 

where \( \tau = |a\beta| \) and \( \phi = \text{arg}(a) - \text{arg}(\beta) \). Eq.(19) tells us that we can simulate the three–body Hamiltonian

\[ H = \lambda \hat{A}\otimes \hat{B}\otimes \sin(\theta \hat{C} + \phi) \]  \hfill (20) 

by the following sequence

\[ \mathcal{D}( -\hat{B}\beta ) R(\theta \hat{C}) \mathcal{D}( -\hat{A}\alpha ) R(-\theta \hat{C}) \times \mathcal{D}( \hat{B}\beta ) R(\theta \hat{C}) \mathcal{D}( \hat{A}\alpha ) R(-\theta \hat{C}). \]  \hfill (21) 

Therefore the ‘nonphysical’ three–body interaction is exactly achieved by eight two–body physical interactions.

Specifically we obtain the Hamiltonian

\[ H = \lambda \hat{A}\otimes \hat{B}\otimes \sin(\theta \hat{C}). \]  \hfill (22) 

If we make a small rotation, i.e., the angle \( \theta \) is small enough, we can approximately realize the three–body interaction Hamiltonian

\[ H = \lambda' \hat{A}\otimes \hat{B}\otimes \hat{C}. \]  \hfill (23) 

among three operators \( \hat{A}, \hat{B}, \) and \( \hat{C} \), where \( \lambda' = \lambda \theta \). Remarkably for some operator \( \hat{C} \) we can even exactly realize the three–body interaction.

Let us consider an operator \( \hat{C} \) which satisfies either \( \hat{C}^2 = 1 \) (self-inverse operators) or \( \hat{C}^2 = \hat{C} \) (idempotent operators). For such an operator we have \( \sin(\theta \hat{C}) = \sin(\theta \hat{C}) \). Therefore Eq.(22) shows that we can exactly realize the Hamiltonian \( \hat{A}\otimes \hat{B}\otimes \hat{C} \). The self–inverse operators we often encounter are Pauli operators and parity operators \( \eta \). Many quantum gates in quantum computer are also self–inverse, such as Hadamard gate, controlled–NOT gate \( (\text{CNOT}) \) \([34]\), SWAP gate and Toffoli gate \([38]\). Examples of idempotent operators are of course given by projection operators.

Summarizing the three–body interaction Hamiltonian \( \hat{A}\otimes \hat{B}\otimes \hat{C} \) is approximately simulated for any operators \( \hat{A}, \hat{B}, \) and \( \hat{C} \), and is exactly simulated if one of the operators is self–inverse or idempotent. For the case of \( \hat{A} = \hat{B} = \hat{C} = J_z \), we approximately have the Hamiltonian \( J_z\otimes J_z\otimes J_z \). By choosing the self–inverse \( \hat{C} = \sigma_z \), we exactly have the Hamiltonians \( J_z\otimes J_z\otimes \sigma_z \), and \( \sigma_z\otimes \sigma_z\otimes \sigma_z \).

Both Eq.(14) and Eq.(21) correspond to a close loop (a parallelogram) in phase space. Now the resulting geometric phases are dependent on a product of commuting operators, which are just the desired simulated Hamiltonians.

**C. Many–body interactions of qubits**

In this subsection we address the simulation problem of some many–body interactions of qubits which are related to quantum spin models in condensed matter theory. From Eq.(20) we have the Hamiltonian

\[ H_c = \lambda \cos(\theta J_z), \]  \hfill (24) 

\[ H_s = \lambda \sin(\theta J_z). \]  \hfill (25) 

Let \( \theta = \pi \) we obtain

\[ H_c = \lambda \cos(\pi N/2) \sigma_0 \otimes \sigma_0 \otimes \ldots \otimes \sigma_0, \]  \hfill (26) 

\[ H_s = \lambda \sin(\pi N/2) \sigma_0 \otimes \sigma_0 \otimes \ldots \otimes \sigma_0. \]  \hfill (27) 

From Eq.(20) with even \( N \) and Eq.(27) with odd \( N \), we can simulate, for arbitrary \( N \), the multi–qubit Hamiltonians.
\[ H_{\alpha \pm} = \pm \lambda \sigma_{\alpha} \otimes \sigma_{\alpha} \otimes \cdots \otimes \sigma_{\alpha}, \]  

The above many-body Hamiltonians are very useful. For instance, let the initial state the \( N \)-qubit system be \( |0\rangle^\otimes N \) and evolve according to the Hamiltonian \( H_{x+} \), then the state vector at time \( t \) is easily obtained as

\[ |\theta, N\rangle = \cos(\theta)|0\rangle^\otimes N - i \sin(\theta)|1\rangle^\otimes N, \]

where \( \theta = \lambda t \). The state \( |\pi/4, N\rangle \) is a multipartite entangled state, which is known to play an important role in quantum information theory.

From Eq.\((28)\), we have the Hamiltonian \( \sigma_{1\alpha}\sigma_{2\alpha}(\alpha = x, y, z) \) for \( N = 2 \), which are just the Ising interactions. As \( \sigma_{1x}\sigma_{2z}, \sigma_{1y}\sigma_{2y}, \) and \( \sigma_{1z}\sigma_{2z} \) commute with each other, we may simulate a general two-qubit Heisenberg model 

\[ H = \lambda_x \sigma_{1x}\sigma_{2x} + \lambda_y \sigma_{1y}\sigma_{2y} + \lambda_z \sigma_{1z}\sigma_{2z}. \]

For \( N > 2 \), i.e., the many-body case, we already have the Hamiltonians \( \sigma_x^\otimes N, \sigma_y^\otimes N, \) and \( \sigma_z^\otimes N \), which satisfy the commutation relations

\[ [\sigma_x^\otimes N, \sigma_y^\otimes N] = iN [1 \pm (-1)^N] \sigma_z^\otimes N. \]  

Here the subscripts + and – indicates the anticommutation and commutation, respectively. From the above equation we see that the three operators either commute or anticommute. For even \( N \), any two of the three operators commute with each other. Then we can simulate the following Hamiltonian \( \[33\] \)

\[ H = \lambda_x \sigma_{x}^\otimes (2k) + \lambda_y \sigma_{y}^\otimes (2k) + \lambda_z \sigma_{z}^\otimes (2k) \]

\( (k = 1, 2, 3, \ldots) \).

However for odd \( N \), any two of the three operators anticommute but do not commute with each other. For \( N = 4m + 1 \) \( (m = 0, 1, 2, \ldots) \), from Eq.\((33)\), we obtain

\[ [\sigma_x^\otimes N, \sigma_y^\otimes N] = 2i\sigma_z^\otimes N. \]

Thus the operators \( \sigma_x^\otimes N/2, \sigma_y^\otimes N/2 \) and \( \sigma_z^\otimes N/2 \) realize the \( su(2) \) Lie algebra. For odd \( N = 4m + 3 \) \( (m = 0, 1, 2, \ldots) \), from Eq.\((33)\), we obtain

\[ [\sigma_x^\otimes N, \sigma_y^\otimes N] = -2i\sigma_z^\otimes N. \]

In this case \( \sigma_x^\otimes (2k)/2, \sigma_y^\otimes (2k)/2 \) and \( -\sigma_z^\otimes (2k) \) realize the \( su(2) \) Lie algebra. For even \( N \) we can find three operators

\[ \sigma_x^\otimes (2k)/2, \sigma_y^\otimes (2k-1)/2, \sigma_z^\otimes I^\otimes (2k-1)/2 \]

satisfy the \( su(2) \) commutation relations. These realizations of \( su(2) \) Lie algebras will be used in the later discussions of quantum gates on encoded qubits.

From any set of commuting Hamiltonians \( \{\lambda_i H_i\} \) we can simulate the Hamiltonian \( \sum_i \lambda_i H_i \) since

\[ \exp(\sum_i \lambda_i H_i) = \prod_i \exp(\lambda_i H_i). \]  

Even for noncommuting set \( \{\lambda_i H_i\} \), we still have a chance that a decomposition similar to Eq.\((36)\) exists \[37\]. For instance, the operators in Eq.\((33)\), \( \sigma_x^\otimes N \), act as the encoded Pauli matrices. Then we have the identity

\[ \exp(-i\phi(\cos \theta \tilde{\sigma}_z + \sin \theta \tilde{\sigma}_y)/2) \]

\[ = \exp(i\theta \tilde{\sigma}_z/2) \exp(-i\phi \tilde{\sigma}_x/2) \exp(-i\theta \tilde{\sigma}_z/2), \]

which implies that we can simulate the Hamiltonian

\[ H = \lambda_z \tilde{\sigma}_z + \lambda_y \tilde{\sigma}_y = \lambda_z \sigma_z^\otimes N + \lambda_y \sigma_y^\otimes N. \]

for odd \( N = 4m + 1 \) using \( \tilde{\sigma}_x = \sigma_x^\otimes N \) and \( \tilde{\sigma}_z = \sigma_z^\otimes N \).

**IV. SIMULATION OF QUANTUM GATES**

So far we have showed how to obtain, by cyclic conditional evolutions in phase space, an operator–dependent geometric phase and how to use these operators in order to simulate two–body and many–body interaction Hamiltonians. Now we make use of the above-developed formalism to explicitly construct some important quantum logic gates. We emphasize that the continuous e.g., vibrational degree of freedom is only required during gating and acts like a databus.

**A. Two-qubit gates**

Controlled–NOT gate \( [34] \) and controlled phase gate \( (C_P) [35] \): Let \( \hat{A} = (1 - \sigma_{1z})/2, \hat{B} = (1 - \sigma_{2z})/2, \) and \( \theta = \pi \) in Eq.\((14)\), the controlled–NOT gate is immediately obtained as

\[ C_{\text{NOT}} = \exp \left[ -i \frac{\pi}{4} (1 - \sigma_{1z})(1 - \sigma_{2x}) \right]. \]

The first bit is the control bit and the second is the target bit. Similarly the controlled–phase gate is obtained as

\[ C_P = \exp \left[ -i \frac{\pi}{4} (1 - \sigma_{1z})(1 - \sigma_{2z}) \right]. \]

A simple relation exists between the controlled–NOT gate and the controlled–phase gate,

\[ C_{\text{NOT}} = \exp \left[ -i \frac{\pi}{4} \sigma_{2y} \right] C_P \exp \left[ i \frac{\pi}{4} \sigma_{2y} \right], \]

i.e., they differ only by local operations.

SWAP gate: As we can simulate the Heisenberg Hamiltonian \( [10] \), the SWAP gate is easily constructed as

\[ G_{\text{SWAP}} = e^{-i \frac{\pi}{8} (\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z)}. \]
B. Three-qubit gates

Toffoli gate ($T$) \[18\]: Let $\hat{A} = (1 - \sigma_{1z})/2, \hat{B} = (1 - \sigma_{2z})/2$, and $\hat{C} = (1 - \sigma_{3z})/2$, in Eq. (23), the three-bit Toffoli gate is obtained as

$$T = \exp \left[ -i \frac{\pi}{8} (1 - \sigma_{1z})(1 - \sigma_{2z})(1 - \sigma_{3z}) \right],$$

which is also called (controlled)$^2$-NOT (C$^2$NOT) gate and important for universal computation. Note the Toffoli gate is exactly realized since the operator $\hat{C} = (1 - \sigma_{3z})/2$ is a projector. Such a gate can be implemented by constructing appropriate networks of one qubit and two qubit gates [18]. The construction showed here is somehow more direct. Notice also that an alternative way to obtain the Toffoli gate is recently discussed in Ref. [18]. The implementation of the more general (controlled)$^k$-NOT will be discussed in Section V.

Fredkin gate ($F$): Another example of a three qubit gate relevant for QIP is provided by the controlled–SWAP Fredkin gate \[39\]. The following commuting Hamiltonians $(1 - \sigma_{x}) \otimes \sigma_{2x} \otimes \sigma_{3x} (\alpha = x, y, z)$ can be realized exactly \[22\]. Therefore we can simulate the unitary operator

$$F = e^{-i \frac{\pi}{2} (1 - \sigma_{1z})(\sigma_{2x} \sigma_{3x} + \sigma_{2y} \sigma_{3y} + \sigma_{2z} \sigma_{3z} - 1)},$$

which is just the Fredkin gate.

C. Quantum gates on encoded qubits

In order to perform universal quantum computations it is sufficient to be able to make arbitrary single qubit rotations together with controlled–phase gate. For encoded qubits one problem is how to make logical operations \[40\] of them and the above two logical operations on encoded qubits are needed. We will discuss two typical codes: the active error correction codes \[41\] and the passive codes on decoherence-free subspaces \[12\].

First we consider the error correction codes with odd number, the linear codes proposed by Steane \[41\]. He have devised two encoding, the first of which protects only against decoherence

$$|0_C\rangle = \frac{1}{2} (|111\rangle + |100\rangle + |010\rangle + |001\rangle),$$

$$|1_C\rangle = \sigma_x \otimes \sigma_x \otimes \sigma_x |0_C\rangle,$$

The second is capable of decoding with general 1-bit errors

$$|0_C\rangle = \frac{1}{\sqrt{8}} (|111111\rangle + |0101010\rangle + |1001100\rangle + |0011011\rangle + |1100000\rangle + |0100101\rangle + |1000011\rangle + |0010110\rangle),$$

$$|1_C\rangle = \sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x |0_C\rangle.$$

The encoded qubits span a representation space of su(2) Lie algebra generated by the operators $\sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_y \otimes \sigma_z \otimes \sigma_z \otimes \sigma_y$ and $-\sigma_y \otimes \sigma_y \otimes \sigma_y \otimes \sigma_z \otimes \sigma_z \otimes \sigma_z \otimes \sigma_y$. Here $N$ is either 3 or 7. That is to say, these three operators acts on encoded qubits as encoded $\sigma_x, \sigma_y$ and $\sigma_z$. Then we consider the code mapping 1 qubit into 5 qubits presented in Ref. [43]

$$|0_C\rangle = Q|00000\rangle, \quad |1_C\rangle = Q|11111\rangle,$$

$$Q = \frac{1}{4} \left[ I \otimes \sigma_x \otimes \sigma_x \otimes I \otimes I \otimes I \right]_{\text{cyc}}$$

$$-(\sigma_x \otimes I \otimes \sigma_x \otimes \sigma_x \otimes I \otimes I \otimes I)_{\text{cyc}},$$

$$-(\sigma_x \otimes \sigma_x \otimes \sigma_x \otimes \sigma_x \otimes I \otimes I \otimes I)_{\text{cyc}},$$

where the subscript “cyc” indicates that addition of all five cyclic shifts. Obviously the commutators $[\sigma^{\otimes 5}, Q] = 0 (\alpha = x, y, z)$ and then $\sigma_x^{\otimes 5}, \sigma_y^{\otimes 5}$, and $\sigma_z^{\otimes 5}$ \[34\] act as encoded $\sigma_x, \sigma_y$ and $\sigma_z$, respectively.

Now we consider even–number codes in decoherence–free subspace \[12\]. We can have a code of two qubits \[44\]

$$|0_C\rangle = |01\rangle, \quad |1_C\rangle = |10\rangle,$$

and a code of four qubits

$$|0_C\rangle = |0011\rangle + |0110\rangle + |0101\rangle,$$

$$|1_C\rangle = |1100\rangle + |1001\rangle + |1010\rangle,$$

For these two cases, it is easy to see that the two-dimensional subspace span\{\{0_C\}, \{1_C\}\} is decoherence–free subspace. The corresponding encoded Pauli matrices are given by Eq. (35).

The controlled–phase gate for encoded qubits is easily constructed as

$$\tilde{C}_P = \exp \left[ -i \pi \left( \frac{1 - \sigma_x}{2} \right) \otimes \left( \frac{1 - \sigma_x}{2} \right) \right].$$

Explicitly for three–bit code we give the gate as

$$\tilde{C}_P = \exp \left[ -i \pi \left( \frac{1}{4} \sigma_x \otimes I \otimes I + I \otimes \sigma_x \otimes I + I \otimes I \otimes \sigma_x + \sigma_x \otimes \sigma_x \otimes \sigma_x \right) \right]$$

which can be realized by our simulation method. Then we have both the rotations of single encoded qubit and gate $\tilde{C}_P$ for two encoded qubits, which are enough for the quantum computation on the encoded qubits.

V. APPLICATIONS TO QUANTUM ALGORITHMS AND DISCUSSIONS

In this section we show some applications of the simulation schemes discussed so far to the implementation of quantum algorithms.
A. Realization of projectors

Let us consider the Hamiltonian

\[ H_k = \lambda \cos[\theta_k(J_z + \phi_k)] \]  

(52)

Since the Hamiltonians \( H_k \) commute with each other for two different \( k \), we have the sum of them

\[ H = \lambda \sum_{k=0}^{N} \cos[\theta_k(J_z + \phi_k)] \]  

(53)

This Hamiltonian can be obtained by \( N + 1 \) cyclic evolutions in phase space. If we choose \( \theta_k = \frac{2\pi k}{N+1} \), \( \lambda = \frac{1}{N+1} \) and \( \phi_k = N/2 + n \) \((k = 0...N)\), the Hamiltonian becomes

\[ H = \frac{1}{N+1} \sum_{k=0}^{N} \cos \left[ \frac{2\pi k}{N+1} (N - n) \right] \]  

(54)

where \( N = J_z + N/2 \) whose eigenvalues range from 0 to \( N \). From the above equation and using the identity

\[ \frac{1}{N+1} \sum_{k=0}^{N} \cos \left[ \frac{2\pi k}{N+1} (n - n') \right] = \delta_{nn'} \]  

(55)

we obtain the Hamiltonian

\[ H = \delta_{Nn} \]  

(56)

which implies that we have realized the projector \( P_n \) which project the state to the symmetric subspace with excitation \( n \). For instance, for \( n = 0 \) or \( N \), the projectors are just

\[ P_0 = |00...0\rangle \langle 00...0|, \]  

(57)

\[ P_N = |11...1\rangle \langle 11...1|. \]  

(58)

A general Hamiltonian \( F(J_z) \) can be written as

\[ F(J_z) = \sum_{n=0}^{N} F(n - N/2)P_n. \]  

(59)

Since all \( P_n \) commute we can simulate the general Hamiltonian \( F(J_z) \).

Once we have realized the projector \( P_0 \) we can realize any one of \( 2^N \) projectors

\[ P_{a_1a_2...a_n} = |a_1, a_2, ..., a_n\rangle \langle a_1, a_2, ..., a_n| \]  

(60)

in the \( N \)-qubit space, where \( a_i \in \{0, 1, ...N\} \) and the state \( |a_1, a_2, ..., a_n\rangle \) represents that the only in the positions of \( a_1, a_2, \) and \( a_n \) the qubit is in the state \( |1\rangle \) and in the state \( |0\rangle \) in other positions. The projector can be implemented as follows

\[ P_{a_1a_2...a_n} = \sigma_{a_1z}\sigma_{a_2z}...\sigma_{a_{Nz}}P_0\sigma_{a_1x}\sigma_{a_2z}...\sigma_{a_{Nz}}. \]  

(61)

Then we realize all the projectors in the \( N \)-qubit space. This can be understood from a more general point of view \[ \mathcal{R} \]. Suppose we have the Hamiltonian \( H \) and perform unitary operations \( U \) and \( U^\dagger \). Then it follows from the identity \( e^{-iUHU^\dagger} = Ue^{-iT}U^\dagger \) that we can exactly simulate evolution according to the Hamiltonian \( UHU^\dagger \). Now our \( H \) and \( U \) are: \( H = P_0 \) and \( U = U^\dagger = \sigma_{a_1z}\sigma_{a_2z}...\sigma_{a_{Nz}} \).

The projector \( P_{a_1a_2...a_N} \) is very useful. For instance, from \( P_N := |1\rangle \langle 1|^N \), the \( (N+1) \)-bit \( C^N_{\text{NOT}} \) gate, is expressed as \[ \mathcal{R} \]

\[ C^N_{\text{NOT}} = \exp \left[ -\frac{\pi}{2} (P_N (1 - \sigma_{n+1x}) \right] = 1 - P_N + P_N \sigma_{n+1x}, \]  

(62)

which is a natural generalization of the controlled-NOT gate and Toffoli gate to many qubits. Alternatively one can construct the multi-qubit generalization of the controlled-phase gate

\[ U_{P_N} = e^{-i\pi P_N/2} \]  

(63)

Then the \( C^{N-1}_{\text{NOT}} \) gate is easily obtained as

\[ C^{N-1}_{\text{NOT}} = e^{-i\frac{\pi}{2} \sigma_{N}U_{P_N}e^{i\frac{\pi}{2} \sigma_{N}U_{P_N}}. \]  

(64)

So we can straightforwardly implement \( C^{N-1}_{\text{NOT}} \) gate once we have had the projector.

B. Implementation of the quantum amplitude amplification algorithm

In 1997, Grover presented a search algorithm \[ \mathcal{R} \] that identifies the single value \( x_0 \) that fulfills \( f(x_0) = 1 \) for a function \( f(x) \) provided, e.g., by an oracle (all other arguments lead to vanishing values of the function). If \( x \) is an integer on the range between 0 and \( N - 1 = 2^n - 1 \), the search algorithm is able to find \( x_0 \) after on the order of \( \sqrt{N} \) evaluations of the function. Grover’s algorithm has been demonstrated on NMR few qubit systems \[ \mathcal{R} \]. In our previous paper \[ \mathcal{R} \] we have shown how to implement the Grover’s algorithm. In the following we will use our method to implement a general quantum search, which is called quantum amplitude amplification algorithm \[ \mathcal{R} \].

We can write a general quantum search operator \[ \mathcal{R} \] as

\[ Q = Q(A, \chi, \varphi, \theta) = -\lambda S_{\chi}^{\varphi} A^{-1} S_{\chi}^{\theta}, \]  

(65)

which is at the heart of the quantum algorithm. Here \( A \) is any quantum algorithm that acts on the \( N \)-qubit system and

\[ S_{\chi}^{\varphi} = 1 + (e^{i\varphi} - 1) |00...0\rangle \langle 00...0|, \]  

(66)

\[ S_{\chi}^{\theta} = 1 + (e^{i\theta} - 1) \sum_k |\tau_k\rangle \langle \tau_k|. \]  

(67)
The state \(|\tau_k\rangle\) is a marked state and the summation runs over all the marked states. Thus this quantum search is a multi–object search. The quantum algorithm contains a unitary transformation, two phase rotations and the marked states. When \(A\) is the Walsh-Hadamard transformation, there is one marked state, and \(\vartheta = \varphi = \pi\), the quantum algorithm reduces to the usual Grover’s search algorithm.

Now we write the two phase rotation operators \(S^\vartheta_0\) and \(S^\vartheta_1\) as exponential form as

\[
S^\vartheta_0 = e^{i\vartheta|00\cdots0\rangle\langle00\cdots0|}, \quad S^\vartheta_1 = e^{i\vartheta \sum_k |\tau_k\rangle\langle\tau_k|}.
\]

As we have all the projectors \((68)\) and they commute with each other, the two rotation operators are then realized straightforwardly. Therefore the general quantum search algorithm can be implemented. In a recent paper [8] the phase rotation operator \(S^\vartheta_1 = 1 - 2 \cos \vartheta e^{i\vartheta |\tau|\langle\tau|}\) is introduced. This operator can be written as the exponential form as \(S^\vartheta_1 = e^{i(\pi - 2\vartheta)|\tau|\langle\tau|}\) and therefore we can realize it similarly as \(S^\vartheta_1\) and \(S^\vartheta_0\).

A few comments on the above geometric scheme in this paper are now in order. From Eq.\((13)\) it can be seen that we still have freedom to make a generalization as

\[
e^{-i\tau_{jk} A_j A_k \sin(\theta_j \hat{C}_j - \theta_k \hat{C}_k + \phi_{jk})} = \mathcal{D}(A_k \alpha_k e^{i\theta_k \hat{C}_k}) \times \mathcal{D}(-A_j \alpha_j e^{i\theta_j \hat{C}_j}) \mathcal{D}(A_j \alpha_j e^{i\theta_j \hat{C}_j}).
\]

Here \(\tau_{jk} = |\alpha_j \alpha_k|\) and \(\phi_{jk} = \arg(\alpha_j) - \arg(\alpha_k)\). So we can simulate the Hamiltonian like \(A_j A_k \sin(\theta_j \hat{C}_j - \theta_k \hat{C}_k + \phi_{jk})\) which includes for arbitrary commuting operators \(A_j, A_k, \hat{C}_j, \) and \(\hat{C}_k\). Then we further ask if we can exactly simulate the product of three arbitrary operators \(A_j A_k C_l\) or more general one, the product of four operators \(A_j A_k C_l C_m\). The answer seems negative with our scheme. The reason is as follows. The general transformation is given by Eq.\((13)\) with \(\alpha_i \rightarrow \alpha_i A_i e^{i\theta_i \hat{C}_i}\). Then if the transformation \(\gamma\) is cyclic, we obtain a geometric phase factor given by

\[
e^{-i \sum_{j > k} \tau_{jk} A_j A_k \sin(\theta_j \hat{C}_j - \theta_k \hat{C}_k + \phi_{jk})}
\]

Hence we can not exactly achieve the products of three or more commuting operators.

**VI. CONCLUSIONS**

In this paper we have discussed a geometric scheme to simulate many–body interactions and to implement multi–qubit gates. Our strategy is based on conditional cyclic evolutions in the phase space of a continuous quantum variable coupled to discrete systems. The cyclic evolution leads to a conditional geometric phase factor containing the discrete factor. To the use of the reader let us list the main results of this work:

1. We can exactly simulate two–body Hamiltonians like \(A \otimes B\), the three–body interaction Hamiltonians like \(A \otimes B \cos(\theta(\hat{C} + \phi))\), \(A \otimes B \otimes C\) with one of them is self–inverse or idempotent, and many–body Hamiltonians like \(\sigma_\alpha \otimes \sigma_\beta \otimes \ldots \otimes \sigma_\gamma\). Some quantum spin models in condensed matter theory are exactly simulated. We approximately simulated the Hamiltonian \(A \otimes B \otimes C\) for three operators \(A, B,\) and \(C\).

4. We simulate the projectors as quantum Hamiltonians and implement the quantum amplitude amplification algorithm.

In conclusion we would like to stress that, in the simulations discussed in this paper, the Hamiltonians involved are given only by conditional displacement operators and conditional rotation operators. These operators can be realized experimentally, e.g., in ion-traps. Therefore we believe that the simulation strategies discussed in this paper have direct practical relevance.

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[1] R. P. Feynman, Int. J. Theor. Phys. 21, 476 (1982).
[2] Special issue on quantum information, Phys. World 11 33-57 (1998).
[3] S. Lloyd, Science 273 1072 (1996).
[4] H. Rabitz, R. De Vivie-Riedle, M. Motzkus and K. Kompa, Science 288, 824 (2000); L. Viola, S. Lloyd, and E. Knill, Phys. Rev. Lett. 83, 4888 (1999); D. Vitali and P. Tombesi, Phys. Rev. A 59, 4178 (1999); S. G. Schirmer, H. Fu and A. I. Solomon, Phys. Rev. A. 63, 063410 (2001); H. Fu, S. G. Schirmer, and A. I. Solomon, J. Phys. A: Math. Gen. 34, 1679 (2001).
[5] M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information (Cambridge University Press, Cambridge, 2000).
[6] M. Stollsteimer and G. Mahler, Phys. Rev. A 64, 052301 (2001).
[7] J. L. Dodd, M. A. Nielsen, M. J. Bremner, and R. T.
[8] P. Wocjan, D. Janzing and Th. Beth, quant-ph/0106073.
P. Wocjan, M. Rötteler, D. Janzing, and Th. Beth, quant-ph/0109098.

[9] C. H. Bennett, J. I. Cirac, M. S. Leifer, D. W. Leung, N. Linden, S. Popescu, and G. Vidal, quant-ph/0107035.
W. Leung, quant-ph/0107041; G. Vidal and J. I. Cirac, quant-ph/0108076.

[10] H. Chen, quant-ph/0109115.

[11] S. Lloyd, Phys. Rev. Lett. 75, 346 (1995); D. Deutsch, A. Barenco, and A. Ekert, Proc. R. Soc. London A 449, 669 (1995); D. P. DiVincenzo, Phys. Rev. A 51, 1015 (1995).

[12] C. Monroe, D. M. Meekhof, B. E. King, and D. J. Wineland, Science 272, 1131 (1996).

[13] C. C. Gerry, Phys. Rev. A 55, 2478 (1997); C. C. Gerry and R. Grobe, Phys. Rev. A 56, 2390 (1997), 57, 2247 (1998).

[14] G. J. Milburn, quant-ph/9908037.

[15] A. Sørensen and K. Mølmer, Phys. Rev. A 62, 022311 (2000).

[16] X. Wang, A. Sørensen and K. Mølmer, Phys. Rev. Lett. 86, 3907 (2001).

[17] S. Lloyd, quant-ph/0008035.

[18] D. P. Divincenzo, Proc. R. Soc. Lond. A 454, 261 (1998); X. Zhou, D. W. Leung, I. L. Chuang, Phys. Rev. A 62, 052316 (2000).

[19] P. W. Shor, SIAM J. Computing 26, 1486 (1997).

[20] L. K. Grover, Phys. Rev. Lett. 79, 325 (1997); 80, 4329 (1998).

[21] S. Chaturvedi, M. S. Siam and V. Srinivasan, J. Phys. A: Math. Gen. 20, L1071 (1987); R. G. Littlejohn, Phys. Rev. Lett. 61, 2159 (1988); R. Simon and N. Kumar, J. Phys. A: Math. Gen. 21, 1725 (1988); G. S. Agarwal and R. Simon, Phys. Rev. A 42, 6924 (1990); M. Dima, quant-ph/9912047.

[22] A. Luis, J. Phys. A: Math. Gen. 34, 7677 (2001).

[23] M. V. Berry, Proc. R. Soc. London Ser. A 392, 45 (1984).

[24] Y. Aharonov and J. Anandan, Phys. Rev. Lett. 58, 1593 (1987).

[25] P. Zanardi and M. Rasetti, Phys. Lett. A 264, 94 (1999); J. Pachos and P. Zanardi, Int. J. Mod. Phys. B 15, 1257 (2001); J. Pachos, P. Zanardi, and M. Rasetti, Phys. Rev. A 61, 010305(R) (2000).

[26] J. A. Jones, V. Vedral, A. Ekert, and G. Castagnoli, Nature 403, 869 (2000).

[27] G. Falci, R. Fazio, G. M. Palma, J. Siewert, V. Vedral and G. Castagnoli, Nature 407, 355 (2000).

[28] L. M. Duan, J. I. Cirac, and P. Zoller, Science 292, 1695 (2001).

[29] Xiang-bin Wang and M. Keiji, Phys. Rev. Lett. 87, 097901 (2001).

[30] D. M. Greenberger, M. A. Horne, and Z. Zeilinger, Bell’s Theorem, Quantum Theory and Conceptions of the Universe, edited by M. Kafatos (Kluwer Academic, Dordrecht, 1989), p. 69; D. Bouwmeester, A. Ekert and A. Zeilinger (Eds.), The Physics of Quantum Information (Springer-Verlag, Berlin, 2000).

[31] K. Mølmer and A. Sørensen, Phys. Rev. Lett. 82, 1835 (1999).

[32] M. Kitagawa and M. Ueda, Phys. Rev. A 47, 5138 (1993).