Simulating the Physics: 
Quantum Simulations in a Nutshell

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(Dated: March 10, 2018)

Thanks to the developing technique of full control of a quantum system, quantum simulations and quantum computation, firstly put forward by Richard Feynman, are nowadays experimentally feasible to discover new physics in condensed matter physics, AMO physics and chemistry. Quantum simulator can be implemented as a simpler quantum computer or more precisely, analogy one. This review is to briefly introduce the recent progresses in quantum simulations of topological insulators, many body phenomenon, quantum optimal control and some works of mine.

PACS numbers: Quantum Computation, Quantum Control, Circuit Quantum Electrodynamics

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I. INTRODUCTION

Quantum simulators serve as controllable, easily accessible quantum systems to simulate much less controllable large system. Back to thirty years ago, to test quantum description of matter become a challenge to computation physicists. It’s obvious that a large quantum system will consume unaffordable storage. The state is described by exponentially growing numbers of parameters while the scales of the system grows linearly. One possible way to overcome this difficulty is to use approximation method such as quantum Monte Carlo simulations. However, there exists so-called "signed" problem that restricts this efficient method. Another possible way is to use tensor network representation of many body wave function. But it is shown inefficient when treating gapless excitations.

From Richard Feynman’s great insight of the problem[1][2], he proposed a new type of computer: *Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws.* But he was not very specific about how can his quantum mechanical computer function and be realized. About one decade later, an ensemble of qubits serving as universal quantum simulator are proposed by Lloyd. In his scheme, the qubits can be initialized, measured and controlled by some engineering procedure.

The potential platforms for quantum simulations and computations includes defects in solid system(NV center), trapped ions, neutral atoms, cavities, photons, quantum dots, superconducting circuits and Nuclear spins. Based on their different advantages and disadvantages, they can accomplish different types of tasks. For example, because of the scalability of ultra-cold atoms, the platform can be regarded as a good one to simulate many body phenomenon. Due to the progress of controlling quantum states and scaling superconducting circuits, this platform can be reagared as a good one to achieve quantum computation. Other platforms can also find their positions in quantum metrology, quantum sensing, precision measurement, chemistry, biology and medicine.

To prepare ourselves with technique which will not only benefit the physics community but also other perspectives in normal life, we should not be fulfilled by these achievements mentioned above. By comparing the quantum simulation results and some exactly solvable models, we are confident about the quantum nature of the simulator and then we should proceed to build a general quantum computer. By physicists’ efforts and innovations, the quantum computers are supposed to be faster than the summary of the computers all over the world in at least one significant practical problem to show so-called *Quantum Supremacy*.

In general, there is still a long way to go for physicists to build and test a universal computer and apply it in some practical problems. However, quantum simulations of some physics model make great progress. For example, it’s very hard to analytically calculate the properties of many body Hamiltonians with interaction, such as Mott-Hubbard Hamiltonian, t-J Hamiltonian and quantum spin chain Hamiltonian. Many interesting quantum phases, entanglement features and topological properties are hidden deeply in the nature of many-body Hamiltonians. To fully extract informations from those systems requires a simulator of quantum nature.

The paper is organized as below: I will briefly introduce some rather general quantum simulation problems
FIG. 1: Scheme of quantum simulations. The original system in the gray block is less accessible and controllable. A well-defined simulator means that its initial state can be prepared, the evolution of the state can be engineered, and the final state can be measured. After mapping from the original system to the simulator and performing quantum gates, one can extract information from simulator. For the two system obey the same physical law, the information one obtained can be remapped to original system.

in Section II. Then I will focus on quantum simulations of some topological band theory by ultracold atoms and superconducting circuits in Section III. A recent work on qubits control by holonomic quantum gates with transmon qubits is introduced as an example of proceeding from quantum simulator to quantum computer in Section IV.

II. GENERAL IDEAS ON QUANTUM SIMULATIONS

Definition of Quantum Simulations We first consider a less controllable system with Hamiltonian $H_{\text{sys}}$ and denote the states in the target Hilbert space as $|\psi\rangle_{\text{sys}}$. As quantum mechanics tells, evolution operator from the initial state $|\psi(t_0)\rangle_{\text{sys}}$ to the final state $|\psi(t)\rangle_{\text{sys}}$ is unitary and denoted by $U(t,t_0) = \mathcal{T}\{\exp[-i\hbar H_{\text{sys}}(t-t_0)]\}$, where $\mathcal{T}$ is the time-ordering operator. And a more controllable system evolves from $|\psi(t_0)\rangle_{\text{sim}}$ to $|\psi(t)\rangle_{\text{sim}}$ via $\tilde{U}(t,t_0) = \mathcal{T}\{\exp[-i\hbar H_{\text{sim}}(t-t_0)]\}$. Then if a mapping from the original system to the quantum simulator exists, the system can be simulated as shown in FIG 1.

In a more algebraic language, the representation of a simulator Hamiltonian can be constructed as:

$$H_{\text{sim/sys}} = H_0 + H_d(t)$$

$$H_0 = \sum_{i,j,m,n} v^i_j m_n (a_i^\dagger)^m a_j^n$$

$$H_d = \sum_{i,j,m,n} u^i_j m_n (t) (a_i^\dagger)^m a_j^n$$

Where $a_i, a_i^\dagger$ denote bosonic or fermionic annihilation and creation operators, respectively. $H_0$ is the simulator Hamiltonian which is fixed and $H_d$ is the artificial Hamiltonian which can be modulated so the system is more controllable. Most models of the simulators and original systems can be easily represented by this language. To simulate a quantum system, the dimension of the Hilbert space of simulator must be larger than the original system. Then, preserving the commutation relations of $a_i$ and $\tilde{a}_j$, one can take the injection $\vartheta : v(u)_{m,n}^i_j \rightarrow \tilde{v}(\tilde{u})_{m,n}^i_j$.

Classifications of Quantum Simulations There actually exists several types of quantum simulation because the different idea used in modulating the Hamiltonian and simulating procedure. Digital quantum simulation (DQS) only require single-qubit gate and two-nontrivial-qubit gate to achieve quantum simulation. The wave function are encoded by the computational qubits and any complicated many-qubit unitary transformation can be implemented through the application of a sequence of single- and two-notrivial gates. Since DQS has the capability to simulate any unitary transformation, the DQS is universal but not all unitary transformations can be simulated with polynomial resources which led to fidelity problems. Therefore DQS can be only treated as a simpler quantum computation method. The components of these simulator often involve in selecting an effective two-level system to construct a qubit as shown in FIG 2. Because of the large gap between qubit and other energy level, the Markovian approximation is valid and other energy and influence from environment can be treated as damping and dephasing together. In a more specific example, e.g. transmon qubit, I will show how to reduce
crosstalk among subspace and other energy levels using quantum optimal control. Another question is the influence of local perturbation or error induced by uncertainty from controller, e.g laser or microwave generator, which means: $H_d(\Omega(t)) \rightarrow H_d(\Omega(t) \pm \varepsilon)$. Some of them can be avoided by proper choice of quantum gate implementation, as will be shown in section [V].

**Circuit Quantum Simulation (CQS)** is a natural but not universal method in which the simulator mimics another system. An uncontrollable Hamiltonian can be directly mapped to another one which can be controlled to some extent. Unlike establishing units in DQS, we treat AQS as a natural system with effective many-body Hamiltonian. So even if the system is less controllable in some special parameter, the phase transitions under study can be sometimes observed and thus provide the question to several types of many-body phenomenon. In the standard formalism of AQS, one must first find the mapping between targets and the simulator. Finding a mapping seems simpler than obtaining a sequence of gates for a given Hamiltonian. But actually sometimes the finding the correct and clever mapping is complicated and need devising.

### III. ANALOG QUANTUM SIMULATION: A CASE STUDY

I will present a practical example to illustrate the basic idea of analog quantum simulation. I propose an experimentally feasible scheme to observe the Berry curvature and Chern number in a topological transition process, using an artificial three-level atom. The Berry curvature is defined in a two dimensional manifold with an adjustable phase factor. By varying parameters of the system slowly but non-adiabatically, Berry curvature can be measured by dynamic hall effect. The simulation shows a sign reversal of Chern number from continuously changing the phase factor, which indicates special topological transition.

Berry curvature [3], which is analogous to the magnetic field but in a parameter space may contribute a lot to study topological properties and provide a new perspective of gauge field. Based on the concept of Berry curvature, it is discovered that topological invariants such as Chern number exists in many typical quantum systems such as condensed matter, photonics and quantum circuits. [3][6]

Meanwhile, in recent years, Berry curvature is measured by transport methods with solid-states, ultracold atoms and photonics. [7][8] Compared with anomalous transport methods, a circuit quantum dynamics simulator can improve integration and scalability. The advances of a long dephasing time and good controllability lead to a success in measuring Berry curvature and Chern number with an artificial two-level atom made by quantum circuits. [9][12] But lots of related physics remain to be discovered in a reduced 3D Hilbert space, for example, Kagome lattice problem. Motivated by this, we propose a single artificial "\(\Delta\)"-type three-level atom to simulate the Kagome lattice, which shows interesting physical phenomenon such as flat band and topological transitions.

In our scheme, we consider 2D manifold of parameters in addition to the 0D system of a single atom, in order to simulate a long-ordered and ideal Kagome lattice Hamiltonian and obtain Berry curvature and further Chern number. We go beyond level counting method in the Hofstadter spectrum. We use dynamical hall effect of a single atom with varying parameter which has also an intuitive interpretation of simulated Lorentz force in the parameter space in presence of Berry curvature.

We consider a cycle-three-level atom in FIG. 3 with arbitrary transitions permitted. The atom has two ground states, \(|0\rangle\) and \(|1\rangle\) and an excited state \(|e\rangle\). We begin with this Hamiltonian to demonstrate the essential steps to measure Berry curvature:

$$H = \omega_e |e\rangle \langle e| + \omega_1 |1\rangle \langle 1| + e^{i\phi} \cos (\alpha_1 + \alpha_2) |e\rangle \langle 0| + e^{-i\phi} \cos (\alpha_1) |e\rangle \langle 1| + e^{i\phi} \cos (\alpha_2) |0\rangle \langle 1| + h.c.$$  (2)

This system is dependent on three different parameters: \(H = H(\alpha_1, \alpha_2; \phi)\). Under the transformation \(\alpha_{1,2} \rightarrow \alpha_{1,2} + 2\pi\), the Hamiltonian remains invariant. We constrain these parameters in the zone: \(-\pi \leq \alpha_{1,2} < \pi\) and hence the full manifold is torus-like. As discussed in the Appendix, Berry curvature and Chern number are defined in this closed manifold.

Then, the Hamiltonian can be simply diagonalized and

![FIG. 3: An algorithms (Quantum Support Vector Machine) implemented by a sequence of quantum gates. (Digital quantum simulation or quantum computation)](image)

![FIG. 4: Scheme of \(\Delta\)-type atom.](image)
the eigen-energies can be obtained:

\[ E_1 E_2 E_3 = E_1 \cos^2 \alpha_2 + E_2 \cos^2 \alpha_1 + E_3 \cos^2 (\alpha_1 + \alpha_2) + 2 \cos \alpha_1 \cos \alpha_2 \cos (\alpha_1 + \alpha_2) \cos 3\phi \]  

(3)

Where \( E_1 (\alpha_1, \alpha_2) = E (\alpha_1, \alpha_2) - \omega_c E_2 (\alpha_1, \alpha_2) = E (\alpha_1, \alpha_2) \) and \( E_3 (\alpha_1, \alpha_2) = E (\alpha_1, \alpha_2) - \omega_1 \) and \( E(\alpha_1, \alpha_2) \) is the energy. Note that for fixed \( \alpha_1, \alpha_2 \) and \( \phi \), there are three values of \( E(\alpha_1, \alpha_2) \). With the definition of the closed manifold, this can be interpreted as an energy band.

In our scheme, there are some biases in the second and third diagonal matrix element of the Hamiltonian \( \omega_1 \) and \( \omega_c \), respectively. But in a special frame, when \( \omega_0 = \omega_1 = \omega_c = 0 \), from Eq. 3 we obtain:

\[ E^3 = (2t + 1)E + t \cos (3\phi) \]

(4)

The middle band will be flat when the condition \( \phi = \frac{\pi}{6} + \frac{n\pi}{3} \) is satisfied. The upper or lower band will be flat when the condition \( \phi = \frac{n\pi}{3} \) is satisfied. Some special cases are shown in Fig. 5. When \( \omega_1, \omega_c = 0 \), the lower band and mid band can be made fully flat. A small perturbation of \( \omega_1, \omega_c \) lead to dispersive bands but these bands are still relatively flat. By tuning \( \phi \), with \( \omega_1, \omega_c \ll 1 \), finite gaps are opened. When \( \omega_1, \omega_c \) is large enough, the gaps are closed and degeneracy occurs. In our method, we only consider the former case because when degeneracy occurs or the gap is so small, there is large deviations and the method lose its efficiency. [13]

**Mapping to the Kagome Lattice.** In the bosonic representation of the Hamiltonian Eq. 2, it can be written as:

\[ H (\alpha_1, \alpha_2) = \psi^\dagger \left( \begin{array}{ccc} 0 & e^{i\phi} \cos (\alpha_1 + \alpha_2) e^{-i\phi} \cos (\alpha_1) & e^{i\phi} \cos (\alpha_2) \\ e^{-i\phi} \cos (\alpha_1 + \alpha_2) & \omega_1 & e^{i\phi} \cos (\alpha_2) \\ e^{-i\phi} \cos (\alpha_1) & e^{i\phi} \cos (\alpha_2) & \omega_c \end{array} \right) \psi \]  

(5)

Where \( \psi = (\psi_a, \psi_b, \psi_c) \) is the vector of bosonic destroy operator. By inspecting the Hamiltonian above and the Hamiltonian of Kagome lattice, we find that they map to each other by a transformation: \( \alpha_1 \rightarrow -k_2, \alpha_2 \rightarrow k_3, \alpha_1 + \alpha_2 \rightarrow -k_1 \), \( H (\alpha_1, \alpha_2) = -2gH (k_2, g) \). The hopping matrix element and accumulated phase of hopping from one site to the nearest one is denoted by \( g \) and \( \phi \), respectively. \( \omega_1, \omega_c \) denote the anisotropy of the sublattice. [14] [15]

**Topological Invariant.** We now consider how to measure Berry curvature and Chern number directly and apply it to our model to discuss how they change with different values of parameter.

**Experimental and theoretical method.** A time-dependent parameter and a dynamical process are needed to obtain Berry curvature. For instance, we simply set \( \alpha_1 = \alpha_1 (t) = \omega_n^2 t^2 \) to demonstrate the method. The initial state is the \( n \)th eigenstate of the Hamiltonian where \( \alpha_2 \) and \( \phi \) is fixed and \( \alpha_1 (0) = 0 \). Then, the system evolves a certain time \( t_f \) and then a linear response can be measured. The Berry curvature of the point \( (\alpha_1 (t_f), \alpha_2) \) can be extracted by:

\[ \langle F_\mu \rangle_f = \langle F_\mu \rangle_0 + \Omega^\alpha_\mu \lambda \frac{ds_\lambda}{dt} + O \left( \left( \frac{ds_\lambda}{dt} \right)^2 \right) \]  

(6)

Where the generalized force \( F_\mu = -\partial_\mu H \) is along the \( \lambda \) direction and the velocity of the change in the parameter is along the \( \mu \) direction. We denote \( (\alpha_1, \alpha_2) \) by \( \vec{s} \). The expectation \( \langle \ldots \rangle_f = \langle \psi (t_f) \ldots (t_f) \rangle \) where \( \psi (t_f) \) is the final state after an evolution due to parameter varying. [13]
For the same original parameters, \( \langle F_\mu \rangle_0 \) is fixed. One can plot \( \langle F_\mu \rangle \frac{d}{d\mu} \) curve and the slop is Berry curvature. We note that by using the dynamic hall effect to measure Berry curvature, the quench velocity is turned on smoothly and the system is prepared in a initial state with large gap.

To justify the measurement of Berry curvature, one can numerically calculate it by the definition like Eq ?? but derivatives of state vectors are used. For the Hamiltonian is not analytically diagonalizable, numerical simulation creates discrete state vectors. By insert the iden-

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The interacting system can be written as

$$H_2 = \sum_{i=1}^{2} \tilde{g}_i (e^{-i\varphi_i} |1\rangle_i |0\rangle_i + H.c.),$$

where $\tilde{g}_i = \sqrt{2}g_i\Omega_i\alpha/|\Delta(\Delta - \alpha)|$ and \varphi_i being the initial phase of the microwave driving field on ith qubit. As shown in FIG.9 the rising time of the pulse $\Delta t$ is $\frac{1}{4}T$ and the effective interaction strength is $\tilde{g} = 10$ Mhz. Our implementation can achieve more than 90% fidelity rate and become a good platform for digital quantum simulation.

V. CONCLUSION

In this review of quantum simulation, I discuss on two type of quantum simulation problem briefly. The main problem of analog quantum simulation is how to map the original system to our quantum simulator, as a kind of solution illustrated by topological insulator. The main problem of digital quantum simulation is how to control the quantum simulator and achieve higher fidelity of quantum gates, as a kind of solution illustrated by holonomic quantum gates with transmon qubits.


