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LDRD PROJECT TITLE:

Noise, Decoherence and Errors from Entanglement-function Theory for Quantum Computing

PROJECT TEAM MEMBERS:

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ABSTRACT:

A significant problem in quantum computing is the development of physical realizations of algorithms that are robust against noise. One way to examine and mitigate noise would be to simulate large sets of qubits coupling to the external environment on classical computers. This is extremely challenging as quantum information processing is in some sense tied to computing resources that scale exponentially with the number of computing elements (qubits).

In this LDRD, we set the foundation for a computational framework potentially allowing simulations of 1000s of qubits vs. 10s now possible. Exact wave-function-based methods demand exponentially increasing resources with system size. The method proposed, entanglement-functional theory (EFT), requires vastly fewer resources. The crucial step is to map the information contained in the wave-functions into a simpler object with associated 1.) auxiliary gate operations and 2.) entanglement functionals of this object. This is similar to the Time-dependent Density Functional Theory (TDDFT) approach that has revolutionized chemistry and materials science. Instead of dealing with the exponentially large wave-function, EFT works with a polynomially large set of projections (the density) that are easily manipulated through unitary operations. For a given set of quantum gates, an isomorphism exists that relates the sequence of events to the time-dependent density. A system of entangled qubits can be simulated at drastically reduced cost relative to existing state-of-the-art vector-state simulation codes.

Once mature this approach may enable 1000 qubit simulations with an explicit treatment of environmental effects. While the method under investigation is currently restricted to closed systems (i.e., strictly unitary evolution) we anticipate being able to generalize our approach to more general open systems. This approach will be possible once reasonably accurate density functionals have been identified and massive simulations can be done. The study of noise and decoherence is crucial for testing proposed noise tolerant algorithms and for assessing their feasibility in physical devices.

INTRODUCTION:

In theory quantum computers offer the possibility of solving certain problems algorithmically faster than classical computers, but the development of practical devices

remains an open challenge due to the need to mitigate noise and decoherence. A key element in practical implementation is the choice of error correction scheme. Without a working quantum computer, these algorithms could be tested in simulators run on classical computers. Simulating a quantum computer on a classical one is an extremely difficult problem and is equivalent to solving the time-dependent Schrödinger equation. Existing simulators for multi-qubit systems rely on schemes that time evolve exact representations of the wave-function or some reduced version of it. Generically these schemes scale exponentially with the number of qubits involved and quickly become too expensive to run on even the largest supercomputers. This problem is the same one that plagued materials and chemical physics for a good part of the 20th century. One extremely efficient and formally exact tool to address this is time-dependent density functional theory. In this theory, the key object that is simulated is some time-dependent density that couples directly to a perturbing field. For systems of interest in chemical and materials physics, this is the electron density, which couples directly to an impressed electrostatic potential. All quantities that could be derived from a wave-function theory can be extracted – albeit sometimes in non-trivial and unknown ways – from the density [10,11,12].

In this LDRD, we advanced the goal of a first of its kind EFT code to simulate qubits. Recent work by Aspuru-Guzik et al. [6] shows a DFT-like theory of qubits is possible and that a non-local functional returns entanglement properties. The main challenges of EFT of qubits are: 1. Finding the effective Hamiltonian. Recent work on Hubbard models suggests that TDDFT of models provides realistic physics of larger numbers of sites than previously possible with wave-function methods [1,3]. 2. Extracting entanglement metrics from the time-evolved local variables. This will involve a nonlocal functional in space and time but at least one such functional has already been found. The work requires the development of a first of its kind EFT code.

This work differs radically from existing approaches in: 1. it is based on an entirely different paradigm and 2. it allows simulations of larger numbers of qubits than previously accessible. Previous approaches rely on statistical or analytic models of states that are intrinsically numerically expensive to compute and store. The EFT approach focuses on the measurement process as the quantity of merit allowing the dynamics of the quantum state to be represented in compact ways and providing a perspective that intimately ties with the inclusion of noise and decoherence in observables.

DETAILED DESCRIPTION OF EXPERIMENT/METHOD:

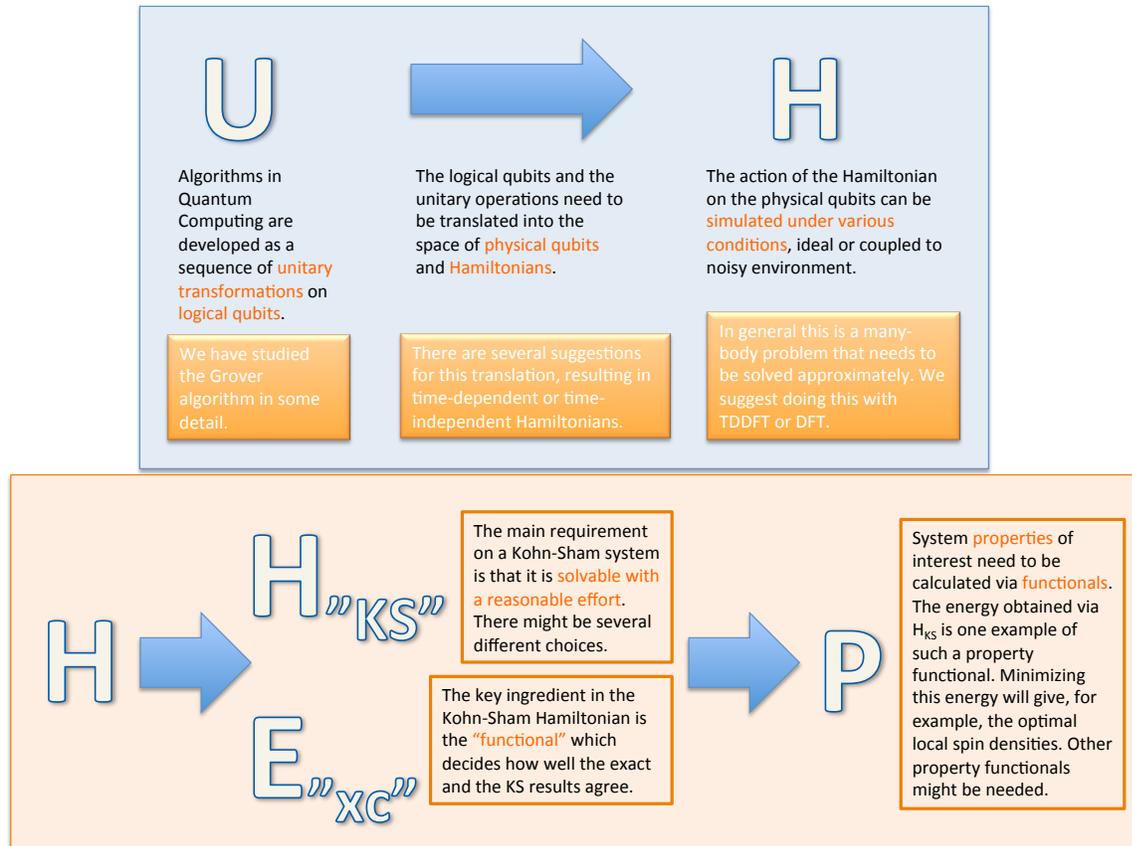


Figure 1: The two major necessary steps we need to take in order to be able to make realistic simulations of how quantum computing algorithms perform in real systems. We first need to find the Hamiltonian that performs the necessary unitary gate operations upon time integration. This Hamiltonian can be time-dependent [2], or time-independent [4]. The next step is to solve the problem defined by this Hamiltonian. In general this will be at least a 2-local Hamiltonian for which the associated Schrödinger equation is difficult to solve. We suggest using the (TD)DFT approach: mapping to an auxiliary Kohn-Sham (KS) system that can be solved generally with less effort than the original problem. The KS Hamiltonian is approximated via parameterizations in terms of densities of exact solutions of special cases.

Time-dependent density functional theory offers an alternative approach to solving the many-body time-dependent Schrödinger equation in the presence of interactions. This is useful for quantum computing simulations because the application of a sequence of unitary gate operations to a system of qubits is identical to the evolution of that system under the action of a time-dependent Hamiltonian[2]. Many of the practical challenges of creating a quantum computer lie in the details of the underlying Hamiltonian. In general, the computational cost of exactly representing a many-qubit wave-function scales exponentially with the number of qubits involved. DFT methods circumvent this issue by mapping the original problem to one that has an auxiliary system with an

efficiently representable wave-function. The cost of this reduction is that the mapping requires an unknown functional that must in practice be approximated. The basic concepts of DFT are expounded in the lower part of Fig. 1. Decades of experience indicate that it is possible to construct accurate approximate functionals for chemical Hamiltonians [9] as well as lattice Hamiltonians of relevance to quantum information processing [1,3].

Much of the success of DFT and TDDFT has been in modeling chemical and materials systems. However, the basic existence proofs that underpin the method also apply to the quantum systems that are being considered for quantum qubits. For example, the always-on Heisenberg model with z -directed control pulses on single qubits can be shown to describe a universal quantum computer [2]. Aspuru-Guzik and coworkers have developed a TDDFT theory that allows one to use simpler spin models to simulate the time evolution of such a system. While much of the literature on DFT is focused on materials and chemistry problems, where the theory has had a profound impact, a budding branch of the theory has focused on model Hamiltonians and cases of strong correlation where available DFT methods were expected to fail. Surprisingly, DFT models often work much better than expected for these systems for reasons that are still being explored. Since the use of an approximate functional in TDDFT is an uncontrolled approximation, it is important to develop DFT methods in cases where exact results are available so that the fidelity of the method can be understood. In our case, this is the always-on Heisenberg model of quantum computation.

The basic Hamiltonian for this model is

$$\hat{H}_0 = \sum_{\langle ij \rangle} J_{x,ij}^\perp \hat{S}_x(i) \hat{S}_x(j) + J_{y,ij}^\perp \hat{S}_y(i) \hat{S}_y(j) + J_{z,ij}^\parallel \hat{S}_z(i) \hat{S}_z(j) \quad (1)$$

where $\langle ij \rangle$ denotes a sum over nearest neighbors; $J_{\{x,y,z\}}$ are the (exchange) interactions between spins, which, if they are unequal, makes the model anisotropic and, in principle could be dependent on the sites i and j . We denote S for the on-site spin, which can be more general than the spin $1/2$ often considered in spin models. The time-dependent control pulses cause the action of unitary gates. These pulses are generically of the form:

$$\hat{H}_{int}(t) = \sum_{i=1}^N h^{ext}(i,t) \hat{S}_z(i) \quad (2) \text{ where}$$

$h^{ext}(i,t)$ are time-dependent local fields coupling to the z -component of the spin. Unitary operations are the result of propagating with the always-on Hamiltonian and the control pulses for a given time-span:

$$U = \exp\left(i \int_{t_0}^{t_1} dt \hat{H}(t)\right)$$

In this LDRD, we have developed the ideas of TDDFT qubits further by

1. Representing a Grover's algorithm through a series of time-dependent pulses,

2. Applying a TDDFT inspired method to a system of two and three qubits,
3. Reproducing Aspuru-Guzik's results and generalizing to more qubits than three,
4. And by considering the challenges of using a z -only perturbation to affect unitary transformations.

We label this approach as EFT rather than TDDFT of Qubits. The first reason is that we are considering Hamiltonians that differ from the many-electron Schrödinger equation for Coulomb interactions. The functionals we use will thus be substantially different from the one's used in materials and chemical physics. The second reason is that many of the quantities of interest to a quantum algorithms developer will involve quantities that are not trivially extracted from the density of the system; thus, a great deal of future work must be devoted to the design of functionals to extract entangled quantities.

RESULTS:

In the first part of this demonstration, we explored the potential of creating a minimal KS representation of a very general multi-qubit Heisenberg model. In this case, we imagined that the control pulses could induce multi-qubit interactions and arbitrary-direction single qubit operations. Such a general model is capable of producing universal quantum computation, and control pulses can be written down readily. This offers a first example of how a complicated multi-qubit simulation can be reduced to a much simpler problem. The KS analogue is a set of single qubit systems each being controlled by x -direction pulses but constrained by the expectation value of the z spin. This systems lies outside the TDDFT proof designed by Aspuru-Guzik, but still lies within the more general framework of TDDFT.

The Grover algorithm requires 3 principle unitary operations: 1. The Walsh-Hadamard transform, 2. an inversion operation, and 3. a diffusion operator. We can write these down explicitly for a two qubit system:

$$\hat{H}_Q = \frac{\pi}{4} (I + \hat{\sigma}_z(1)\hat{\sigma}_z(2) + \hat{\sigma}_z(1) + \hat{\sigma}_z(2))$$

$$\hat{H}_N = \frac{\pi}{4} (I - \hat{\sigma}_x(1)\hat{\sigma}_x(2) + \hat{\sigma}_x(1) + \hat{\sigma}_x(2))$$

Along with the single qubit flip operation:

$$\hat{H}_{P(i)} = -\frac{\pi}{2} \hat{\sigma}_x(i)$$

Since functionals do not exist for this model, we started by using the simplest approach assuming that each qubit only knows about the expectation value of the others spin and only at an instant in time. This is the adiabatic approximation. We then modify the many qubit pulses to reflect this.

$$\hat{H}_{Q(i)} = \frac{\pi}{4} (I + \hat{\sigma}_z(i)\langle \hat{\sigma}_z(i+1) \rangle + \hat{\sigma}_z(i)) ,$$

$$\hat{H}_{N(i)} = \frac{\pi}{4} (I - \hat{\sigma}_x(i)\langle \hat{\sigma}_x(i+1) \rangle + \hat{\sigma}_x(i)) ,$$

$$\hat{H}_{P(i)} = -\frac{\pi}{2} \hat{\sigma}_x(i)$$

In many ways, this is equivalent to Thomas-Fermi theory of electrons in which we only retain obvious information about the density in our functional design. We see that even at the level of this crude model, we can reproduce reliable results for some routes of the Grover algorithm. Note that for the Grover algorithm, the final state is characterized by the set of spin expectation values on the qubits. We do not need any special entanglement functional. This is a special case and will not be true in general. Figure 2 shows the result of applying a series of pulses tailored to the Grover algorithm for a two and three qubit system.

We can also introduce a small level of disorder in our J couplings and find that the result is not significantly altered. Thus, we have reduced the exact exponentially scaling problem to an approximate one that scales linearly. However, accurate functional design in this case is probably not possible. For three qubits for example, we need $2^3=8$ states for the exact solution and $3 \times 2 = 6$ for the TDDFT solution. However, in the exact case, the wave-function at the previous time step and the time-dependent Hamiltonian determine the wave-function at the next step. In TDDFT, the entire history of the spin expectation values determine the solutions.

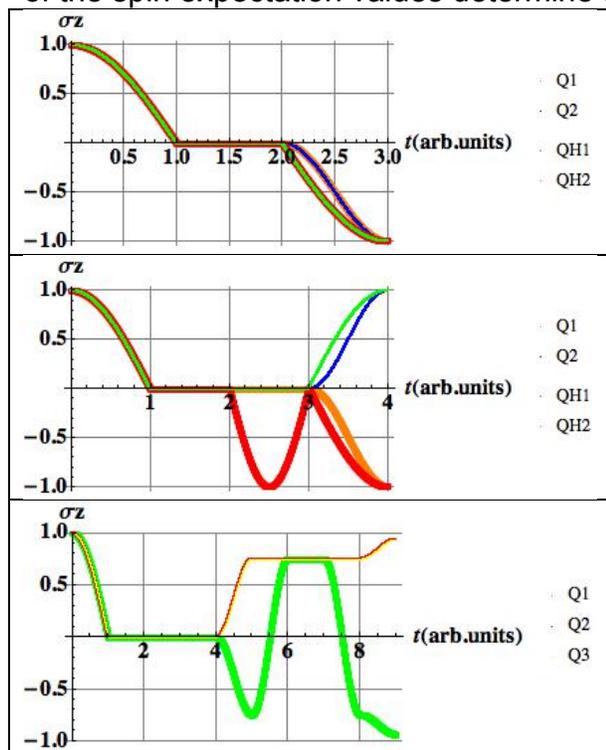


Figure 2: z-spin expectation values over time as the Grover algorithm is applied on a Heisenberg model. The top two panels are 2 qubit systems, and the bottom one is for 3 qubits. The exact results track the TDDFT ones closely.

The power of Aspuru-Guzik's approach is that it retains explicitly multi-qubit couplings in the KS system. This is important to developing accurate approximate functions, much like the difference between orbital-free and orbital-based DFT. We have implemented the method and have generated results for 8 qubits. See Figure 3. We see that we can

represent the same dynamics using a general but intractable XXZ Heisenberg Hamiltonian with a more tractable XY model. This result illustrates that DFT is possible because we can represent 2 very different interaction types in our Hamiltonians that give the same observables. We did this by inverting exact results to find the KS ones. However, the utility of this approach so far is limited because we did not create any model of an approximate potential. Additionally, this method relies on the control pulses being only in the z -direction. It is possible to simulate universal quantum computing in this fashion but auxiliary qubits are needed as the entire quantum simulation must occur in a degenerate subspace of the full Hamiltonian.

We evolved an 8 qubit ferromagnetic Heisenberg XXZ model with sinusoidal local fields with phase alternating by site. Using the TDDFT scheme outlined by Tempel, we extract local control fields for an 8 qubit antiferromagnetic XY model that reproduce the site densities of the Heisenberg system. The results illustrated in Figures 3 and 4 start from a normalized random initial state in which the amplitude of each state in the computational basis is drawn from independent identically distributed Gaussian random variables with mean zero. It is interesting to note that our scheme can resolve time-evolving kinks in the local density and the necessary sharp features in the corresponding local control fields in the auxiliary (XY model) system.

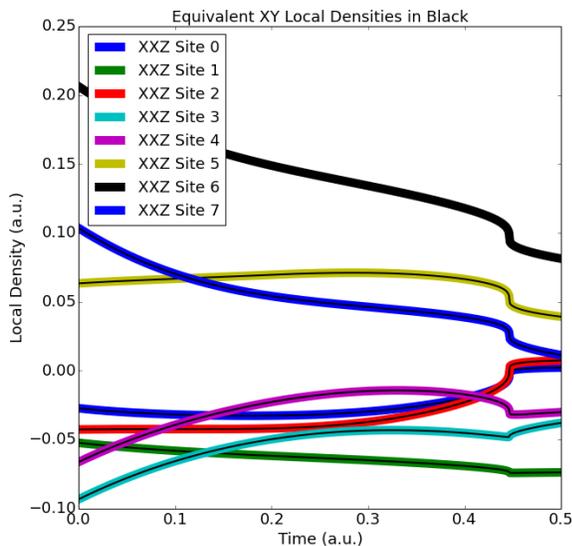


Figure 3: The local densities of the time-evolved XXZ system are illustrated in color for the conditions described in the text. The equivalent local densities in the auxiliary XY system are shown as black lines tracking these densities. This illustrates that we can find local fields that reproduce sharp dynamical features in the XXZ system using TDDFT, such as those ~ 0.44 a.u. into the evolution.

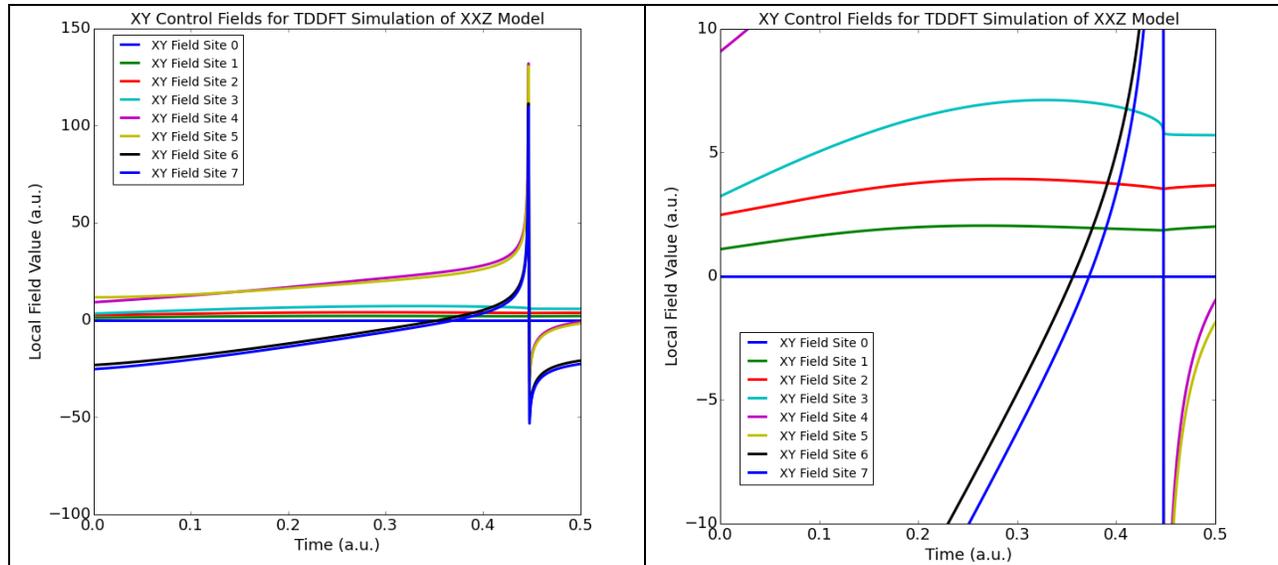


Figure 4: The control fields in the XY system that reproduce the XXZ evolution shown in Figure X showing the full range of the potential and zoomed in for more detail. Here it is evident that the TDDFT potential evolves very sharp features in response to sharp changes in the local densities.

Despite the success shown, several challenges remain:

1. The limitations of the always-on z -perturbation Heisenberg model
2. The role of non-adiabatic effects in functionals
3. The development of entanglement functionals. The latter was not investigated in this effort.

The last two must be addressed in future research efforts. The first one is the result of restricting to a degenerate subspace of the Heisenberg Hamiltonian. This is really only an issue if we want to represent a minimal quantum circuit in which every qubit represents a logical qubit. It is unlikely that any practical quantum computer will have this structure, but from a circuit modeling point, the equivalence is satisfying. On the other hand, using the always-on z -pulse Heisenberg Hamiltonian requires vastly more physical qubits than logical qubits and involves the manipulation of potentially redundant information.

DISCUSSION:

It has been shown that the unitary transformations necessary in quantum computing algorithms can be mapped onto the anisotropic Heisenberg Hamiltonian [2] with external local fields as in the equation above (see also Figure 1). The time-dependent system formed by combining Eqs. (1) and (2) is the starting point for our further elaborations.

Klaus Capelle pioneered the field of Density Functional Theory (DFT) methods for

model Hamiltonians like the one in Eqs. (1) and (2). In his extensive and recent review article [3], he discusses no less than two possible KS systems with corresponding Local Density Approximations (LDAs) [1,5]. One of the schemes takes the large spin view which results in

$$\hat{H}_{KS} = \sum_{\langle ij \rangle}^N J(i,j) (S_x(i)S_x(j) + S_y(i)S_y(j) + \Delta S_z(i)S_z(j)) + \sum_{i=1}^N h^{ext}(i,t)S_z(i) + E_c[\{J(i,j)\}, \Delta; \{S_{\{x,y,z\}}(i)\}] \quad (3)$$

where $S_{\{x,y,z\}}(i)$ are the components of *classical* spin vectors, $J(i,j)$ is the interaction between spins at site i and j , and Δ can make the model anisotropic if different from 1, and the correlation energy functional, E_c , needs to be approximated.

There are several LDA-type functionals derived for this KS system. The key is to solve the exact Hamiltonian formed by Eqs. (1) and (2), for a uniform system, subtract the first part of the KS Hamiltonian in Eq. (3) for the same system, and parameterize the remainder in terms of the parameters of the uniform system. A uniform system has $J(i,j) = J$ and all spins have the same magnitude S . The exact Hamiltonian can be solved approximately with, for example, non-linear spin-wave theory or Density Matrix Renormalization Group methods and the first part of the KS Hamiltonian yields the Néel state with well-known energies in terms of J , Δ , and S . These classes of methods we call *classical spin KS*.

These LDA-type functionals have been applied to inhomogeneous systems with various boundary conditions and impurities, such as one $S = 1$ impurity in a $S = 1/2$ chain. Inhomogeneities due to variations in interaction strength can also be addressed but have been less successful with currently available functionals.

The other KS system, *XY model KS*, discussed in Capelle's review [3] is the XY model derived from the specialization of Eqs. (1) and (2) to the XXZ quantum spin-1/2 chain [1], also discussed and generalized by Tempel and Aspuru-Guzik in Reference [6]:

$$\hat{H}_{KS} = \sum_{\langle ij \rangle}^N \frac{J'(i,j)}{4} (\hat{\sigma}_x(i)\hat{\sigma}_x(j) + \hat{\sigma}_y(i)\hat{\sigma}_y(j)) + \sum_{i=1}^N \frac{h^{eff}(i,t)}{2} \hat{\sigma}_z(i) \quad (4)$$

where $\hat{\sigma}_{\{x,y,z\}}$ are the Pauli matrices coming from the spin-1/2 relations $\hat{S}_{\{x,y,z\}} = \hat{\sigma}_{\{x,y,z\}}/2$. Note that the correlation energy in this case is included in the new parameters J' and the effective local fields $h^{eff}(i,t)$, much as the non-interacting KS kinetic energy and the effective potential replaces the interacting kinetic energy and the external potential in conventional DFT. The key to using this system as a KS system is that it can be solved for with reasonable computing resources compared to the much more computationally expensive XXZ model [1].

LDA-type functionals for the KS system in Eq. (4) are functions of $\{\hat{\sigma}_z(i)\}$, and can be obtained by parameterizing Bethe Ansatz solutions to the exact Hamiltonian from Eqs. (1) and (2) (with $\hat{S} = \hat{\sigma}/2$) for closed spin-loops of size L with $h^{ext}(i,t) = 0$ in the

thermodynamic limit $L \rightarrow \infty$. An improved functional has been developed by keeping the homogeneous system finite, thus introducing a global variable L into the functional. By introducing an average density $n = \sum_i \hat{\sigma}_z(i)/L$, additional accuracy can be achieved.

We have found that we can invert the exact result to a TDDFT KS system successfully in both situations. Practical schemes require approximate XC functionals. It was not the goal of this proof of principle, information gathering LDRD project to design functionals. The development of functions is complicated effort that requires more resources than were available for this project. A future area of work would be the development of functionals so that the accuracy of practical versions of these algorithms could be assessed.

ANTICIPATED IMPACT:

The impact of this work is the refinement of ideas regarding the development of EFT or a TDDFT of qubits. We have shown that the method is feasible to model a Grover circuit, but much work remains. If we are concerned with a theory of only logical qubits, the always-on Heisenberg model is insufficient and the utility of TDDFT for z -only perturbation models comes into question. If we allow for the possibility of auxiliary qubits, we will certainly need to use a different effective Hamiltonian in practice. A more general TDDFT is still possible, but the development of the theory is in a much earlier stage.

Fifty years of functional development for chemical and materials systems give us some indication of what to expect in creating functionals for qubit Hamiltonians [9]. Experience indicates that there are special challenges attendant to developing approximations for time-dependent DFT – specifically, the effect of non-adiabaticity (i.e., history dependence) [7]. Preliminary results in this report indicate that the spin systems we are interested in will exhibit complicated non-adiabatic effects even when used to simulate relatively simple quantum circuits, such as those required by Grover’s search algorithm.

For the spin models that we are currently studying, only adiabatic – or time-local - functionals have been developed. Specifically, Alcaraz and Capelle have proposed a class of ground state functionals for spin chains based upon a local density approximation [1,3]. These functionals are designed to capture properties beyond simple ground state energetics, specifically critical exponents and conformal anomalies. While they have excellent performance for these properties, it is not yet known how well they will perform within an adiabatic TDDFT. Ongoing work will test these functionals within our recently implemented TDDFT-for-qubits framework. We will be able to quickly assess the performance of these existing functionals and can assess critical deficiencies germane to simulating quantum circuits rather than ground state properties.

An alternative approach to applying existing adiabatic functionals within TDDFT is to reformulate the time-dependent problem in terms of a ground state DFT problem for which the question of adiabaticity is irrelevant. Two key frameworks may enable this program to be carried out – the Feynman clock [8] and ground-state quantum

computation [4]. Recently, the Feynman clock formalism has been shown to be a powerful tool for reframing quantum dynamical problems in terms of a variational minimization, rather than a saddle point problem (e.g., finding stationary points of an action functional). Ground-state quantum computation is a similar technique, in which the usual unitary evolution of a quantum state is encoded in spatially disjoint qubits that represent the state of the system at different effective times. Specific gates are then encoded in the coefficients of a time-independent Hamiltonian. These two frameworks can be investigated as an alternative means of developing an intuition for functional development in Hamiltonians of relevance to quantum computation.

Two classes of functional development must be pursued. A future direction of this work is to develop non-adiabatic functionals for time-dependent models. One approach that would be possible here is a machine learning approach since for small systems exact solutions are possible. It would be possible to use this information to develop functionals that given a time-history of many qubits in the general area of a target qubit could produce a non-adiabatic functionals. Another approach might be a straight-forward generalization of adiabatic functionals with efficiently computable non-adiabatic effects that depend on the history of the average density, with an exponentially decaying memory kernel.

Once suitable functionals are designed, the EFT method will scale favorably so that massive numbers of sites are possible. These calculations could include logical qubits composed of multiple physical qubits that would enable the simulation of error correction schemes. To study the effect of decoherence we might also generalize our approach to include non-unitary evolution by way of applying TDDFT to Lindblad-type equations [13].

While it looks like EFT is indeed a promising avenue for realistic multi-qubit simulations, a great deal of work needs to be done to bring this goal forward. Accurate functionals for both the time evolution and for extracting observables must be developed and tested. We will continue to pursue the development of these ideas in a full LDRD proposal.

CONCLUSION:

In this LDRD, we have shown that EFT is possible for qubits by explicitly inverting exact solutions of the Heisenberg model, an exemplary time-dependent Hamiltonian capable of universal quantum computation. This work builds upon the success of TDDFT for Hamiltonians of interest in chemical and materials physics. To demonstrate that useful algorithms may be performed within this framework, we applied a series of multi-qubit pulses on a Heisenberg model and created a simple KS-like representation through non-interacting qubits. Independently, we implemented Aspuru-Guzik's algorithm for an arbitrary number of qubits demonstrating that we can scale to a larger numbers of qubits than previously reported using an XY model system as the KS system. We also developed pulses that achieve the desired unitary operations on qubits for the always-on Heisenberg model but discuss limitations due to being restricted to a degenerate

subspace of the model. We also considered approaches to approximate functional design in TDDFT. While two KS systems with associated LDA-type functionals have been considered in a different context, more investigations are needed in order to evaluate the applicability for quantum computing applications. While the first *classical spin KS* approach might be limited by the need to include all quantum coherence into the functional, the second *XY model KS* approach might be limited in its ability to treat larger spins and spin impurities and also by its much larger computational cost. It is likely that in both cases improved functionals are needed. It is desirable to also investigate if other KS systems can be found - perhaps among integrable systems that can be studied more easily than the full many-body problem. The challenge of non-adiabatic effects can be addressed in two ways, either by developing memory enabled potentials by examining exact solutions of the Heisenberg model or by exploiting the ideas of converting time evolution into a larger system of qubits and considering the ground state of said system. Future work will investigate both routes.

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