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Quantum Smart Matter

Tad Hogg and J. Geoffrey Chase
Xerox Palo Alto Research Center
3333 Coyote Hill Road
Palo Alto, CA 94304, U.S.A.
hogg@parc.xerox.com, chase@parc.xerox.com

The development of small-scale sensors and actuators allows for constructing "smart matter" in which physical properties of materials are actively controlled in a distributed manner. In this paper, we describe how quantum computers could provide an additional capability, programmable control over some quantum behaviors of such materials. This emphasizes the need for spatial coherence, in contrast to the more commonly discussed issue of temporal coherence for quantum computing. We also discuss some possible applications and engineering issues involved in exploiting this possibility.

1 Introduction

Distributed control using many sensors, computers and actuators, can improve the performance of systems at many scales. Examples include controlling traffic flow in cities [29], regulating office environments [24], active strengthening of structural materials [6], structural vibration control [23], reducing fluid turbulence [7] and adjusting optical responses [31]. The continuing development of micrometer-scale machines [10] and proposals for even smaller devices [19] constructed with atomically precise manipulations [3, 20, 25, 35] offer further possibilities for designing materials whose properties can be modified under program control, giving rise to so-called "smart matter" [26].

Smart matter is a material that locally adjusts its response to external inputs through active control. Such control is enabled by embedding sensing, computation and actuation ability within the material. Specifically, control laws are designed to use measurements of the system response to compute appropriate control inputs, such as forces or electric fields, which are then imposed on the system by the actuators. This operation is known as closed-loop control because the control inputs are determined by feedback from system response measurements. Distributed control in smart matter contrasts with more conventional controlled systems where there is a single, global control mechanism.

There are two primary considerations in the creation of any type of controlled system. The first, is the general type of control method to be employed: global or decentralized. The second, is the behaviors that it is desired to control: classical or quantum. Global control is an extremely well researched field [9, 18, 38, 39] in which the basic methodology requires a single centralized controller that receives measured data, and delivers control inputs. A large majority of the control applications implemented today fall into this category. This approach requires global knowledge of the system to create the controller, which is self-limiting in that control design for large systems becomes mathematically intractable. There is also a communication difficulty of providing all the relevant system measurements to the global controller in a timely manner. Distributed, or decentralized, control systems, consist of controllers that are designed and operated with limited knowledge of the complete system. This approach can allow control to be applied to more complex systems, however, global performance cannot be guaranteed as with global controllers. Some applications include regulating: office environments [24], traffic flow [29], and structural vibrations [23].

The control examples mentioned above all involve acting on classical behaviors. However, small, precisely constructed devices can also exploit quantum behaviors, which is the second consideration mentioned previously. For example, quantum behavior can be engineered through the detailed design of structures [1, 33, 34]. It is also possible to provide global control of quantum systems through the use of external fields or lasers to manipulate the behavior of molecules [14, 40], and adjusting these inputs based on measurements of the system response. However, as with classical systems, global controllers are limited in their ability to rapidly meet a variety of specific local needs in a large system. In addition, designing effective global control becomes intractable due to the difficulty of modelling the quantum behavior of large heterogeneous systems.

Thus, an interesting open question is the extent to which the demonstrated abilities to globally modify quantum behaviors, together with distributed computation, can be used to provide a much finer level of control of the properties of a material. In this context, classical computers have a limited role due to their use of a measurement process which necessarily disrupts the quantum behavior.

Instead, control of the quantum behavior of materials is a possible application for quantum computers [4, 8, 15, 16, 17, 21, 28]. This contrasts with most studies of such machines, with their focus on purely computational questions such as whether they can compute classically intractable functions, although there has been some work on distributed, parallel quantum computers [30]. Quantum computers are distinguished by their ability to operate simultaneously on superpositions of many classical states ("quantum parallelism"), and their restriction to unitary linear operations on such superpositions which can be used to produce interference among different computational paths. In particular, this restricts the programs to be reversible, and hence requires development of reversible devices [32].

In this paper, we discuss coupling the programability of quantum computers to properties of materials, to give quantum smart matter. Both classical and quantum smart matter share the basic idea of using a large number of locally controlled sensors, computers and actuators. However, they differ in that using quantum computers as the controllers avoids the need to perform measurements on the system. In the remainder of this paper, we first present an idealized example, then discuss a number of possible applications.

2 Programmable Quantum Behavior

The most extreme case of smart matter is when the computation needed for the control is fast compared to any relevant changes in the physical configuration of the material. This allows for a decoupling of the slow physical degrees of freedom, which we denote by P, from the rapid computational degrees of freedom, denoted by C, in the same way that molecular or solid-state dynamics can often be approximated by considering separately the behavior of the electrons and the atomic nuclei. For example, this could be achieved by using light particles for the computation while heavy ones determine the relevant physical response. Viewed another way, within a given implementation, this requirement also limits the number of computational steps that the control program can perform to determine its result, thus, defining the maximum desired latency of the control system.

To be used in a control context, the forces acting on the physical degrees of freedom must also depend on the computational ones. This is the analog of actuators in classical smart matter where results of a computation can change the forces acting on the physical system. Thus the potential acting on P must be a function $V(P,C)$. Within the range of variation of this function, the control program can adjust C, based on the value of P, to produce an effective physical potential defined by the equation:

$$V_{\text{eff}}(P) = V(P, C(P)) \qquad (1)$$

Because a quantum computer can perform this operation on quantum superpositions, it can produce a system whose relevant physical behavior is governed by $V_{\text{eff}}(P)$. Note that classical computers won't work at this level of detail since they would require a measurement of the state, hence collapsing the wavefunction.

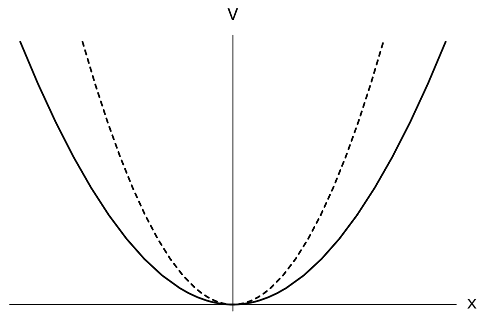

Figure 1: Example potentials $V(x,C)$ for use with quantum smart matter. Two cases, $V(x,0)$ and $V(x,1)$, are shown by the solid and dashed curves respectively, corresponding to a system with two computational states.

For example, consider a one-dimensional system with a single extra binary degree of freedom. In this case the physical degree of freedom is the position, i.e., $P = x$, and the computational degree of freedom C is 0 or 1. A simple potential would be to have two distinct functional forms $V(x,0)$ and $V(x,1)$, as shown in Fig. 1. Suppose the system is initially prepared in the state $|\psi\rangle = \sum \psi(x)|x,0\rangle$ and then acted on by a quantum computer whose program sets C to 0 or 1 depending on whether $x \leq 0$ or $x > 0$, respectively. This gives

$$|\psi\rangle = \sum_{x \leq 0} \psi(x)|x,0\rangle + \sum_{x>0} \psi(x)|x,1\rangle \qquad (2)$$

As this state evolves, amplitudes from positive and negative values of x become mixed and the control computation acts to readjust C. Provided this computation is fast compared to the physical evolution, this gives in effect the behavior governed by the programmed potential. Other effective potentials could be constructed with different programs.

In this example, the result is an asymmetric potential as has been studied in the context of second harmonic generation in optics [34]. This illustrates the trade-off between smart materials and direct construction of materials with the desired effective potential. On the one hand, the properties of smart materials can be readily modified simply by changing the program in the control computers. On the other hand, direct implementation in materials allows for a faster response but becomes more difficult as more complex or time-variable potentials are considered.

As a final comment on this example, note that it made use of quantum parallelism but no use of interference. The latter capability of quantum computers is crucial for their possible improvement on classically intractable problems, and provides additional possibilities for designing behavior of smart matter. For instance, the use of destructive interference could be used to cancel the amplitudes of certain undesirable behaviors, a feature that is not possible with classical computations, even if they are probabilistic.

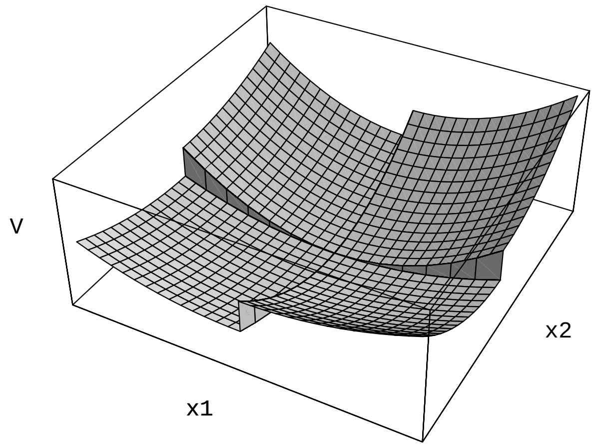

Figure 2: Example potential $V_{\text{eff}}(x_1, x_2)$ obtained from a control program that couples two one-dimensional systems. This potential introduces correlations in the behavior of the two systems.

So far, we have described the behavior of a single quantum controller. For use in smart matter, we would have a system consisting of a large number of such devices to allow distributed control over some quantum behaviors of the material. This can include programs that provide different behaviors at different spatial locations, as well as changing with time. Furthermore, the control computation could make use of some of the computational states of its neighbors, providing a way to build correlations among different regions of the material. An example of how simple programmed couplings can lead to more complex potentials is shown in Fig. 2. In this case, we start with two independent one-dimensional systems whose individual potentials take the form $V(x, C)$ shown in Fig. 1. The overall system potential is then

$$V(x_1, C_1, x_2, C_2) = V(x_1, C_1) + V(x_2, C_2) \qquad (3)$$

We can couple the behaviors together with a control program that, for instance, sets C_1 to 0 or 1 depending on whether the *other* system state satisfies $x_2 \leq 0$ or $x_2 > 0$, respectively, and vice versa for C_2. The resulting $V_{\text{eff}}(x_1, x_2)$ is shown in Fig. 2.

In summary, quantum smart matter relies on potentials that can be adjusted by their dependence on some degrees of freedom that can be rapidly changed under program control. To maintain superpositions, the control computations must rely on quantum computers.

3 Applications and Control

Quantum smart matter consists of actuators, sensors and computers integrated to operate on quantum behaviors, in contrast to the usual emphasis on classical behaviors in smart matter [6, 26]. Intuitively, applying control to quantum behaviors elegantly extends the capabilities of smart materials, since the active elements can operate with the full quantum state of the material. Realizing this possibility requires translating classically based control methods to quantum systems. These methods include closed-loop or controlled behavior based on either feedback or modelling [9, 18, 38, 39]. The difficulty of applying these control techniques will depend to some extent on the way the system is constructed.

At one extreme, precise construction [19] simplifies the control problem by allowing accurate modelling of the environment of each device and individually tailored programs, but imposes severe difficulties for fabrication. On the other hand, more readily manufactured devices will exist in a statistically variable environment, making the control issues more difficult. It is this case that we mainly focus on here, as it raises a number of engineering control issues.

The first, and most obvious, is that creating macro effects with microscopic controllers will require literally billions of these controllers. An immediate consequence is the requirement that these controllers be relatively homogeneous in design and function to simplify their construction. Furthermore each controller will be required to act either autonomously, or in concert with only a few others, since the design of billions of controllers using a global model and algorithm becomes intractable. Thus, an immediate conclusion is that quantum smart matter be based on controllers, designed with local knowledge and behavior, which are homogeneous and act autonomously to achieve a desired macro effect.

A secondary result of this observation is that global simulation and performance predictions will be statistical in nature due to the inability to pinpoint position, or perform simulation and optimization for billions of discrete variables. That is, location of the devices would be described according to a probability distribution rather than known a priori, as assumed by standard control methods. This fact will require different types of systems analysis than are typically employed with classical systems.

A second, equally important, issue is that of stability, the ability of controllers to achieve the desired macro result in the presence of perturbations or uncertainties. Here it is important to note that each individual system has an open loop, or uncontrolled, potential $V(P, C)$, and a closed loop, or controlled, potential $V_{\text{eff}} = V(P, C(P))$ as defined in (1). Applying standard system analysis methods [9, 18, 38, 39], it is straightforward to note that if V_{eff} is convex and has a non-positive total derivative with respect to time (i.e., including the time dependence introduced by adjustments made by the control program based on changes in the system state), then the entire system under consideration will be stable in the closed loop state. This result suggests a direct link between the quantum potentials $V(P, C)$, and standard control theory in which there are several synthesis methods which guarantee stability and performance of the closed loop system. Such synthesis techniques would be employed to design the control program acting on C such that it is reversible and satisfies the stability conditions for $V_{\rm eff}$. Thus, closed loop stability could be guaranteed for individual systems employing appropriate (convex) potential functions. However, it is important to note that stability of each individual system does *not* guarantee stability of the entire macro system under consideration, unless each system is entirely autonomous.

The above results indicate that while design, and synthesis of individual controllers may be put into a form which guarantees local stability and performance, global stability is not as straightforward a problem. Such global stability measures would likely differ from those of standard control theory in being a statistical expectation of stability, rather than a specific proof. Stability in this sense is particularly desirable under the assumption that the undesirable interaction of enough elements could reduce the expectation of stability for the entire macro system, and introduce undesirable behavior. Hence, the interactions present at the microscopic scale to which control is being applied would have to be determined or estimated, because the application of localized controllers to achieve global results is inherently affected by the strength of (potentially) unmodelled interactions.

The final issue involves the construction of the devices. While some progress has been reported on the basic components of quantum computers [2, 13, 37], quantum smart matter also requires sensing and actuation abilities that can be coupled to such computations. Thus progress in the development of quantum based sensing and actuation is needed before applications, such as those presented in this paper, become possible. In addition, it is also important to understand the relative time scales possible for quantum computing and various physical behaviors that might be controlled. This knowledge is required to develop effective sensing and actuation mechanisms for any particular application. Only when the computing is relatively fast can we hope to construct smart matter for the behavior in question.

To illustrate the concept of quantum smart matter, for active control, several potential applications are presented. All of these examples are based on applying microscopic decentralized or local control to create a desired macro result. A brief listing of these applications includes: active camouflage; custom manipulated material properties; active control of certain chemical reaction rates; and nonlinear, active springs for quantum machines.

The key idea is to be able to operate on the full quantum state through program control so as to produce a desired behavior. In some cases, this will amount to adjusting the amplitudes of various states to achieve a high probability of a desired configuration.

3.1 Active Camouflage

The active camouflage idea takes advantage of the ability to create asymmetric, optical potentials within materials [34]. Manipulating these potentials allows the controller to manipulate the optical response to light striking that material and, thus, for example, change the color with which it appears to an external observer. This would allow quantum smart matter to determine the color of its exterior surroundings, and modify the material potentials to reflect a matching color. The end result is a material capable of actively blending in with its surroundings like a chameleon.

There are several different time scales involved in this example. First is the fast interaction of light with the material. This is likely to be much faster than the time scale governing computational speed. However, for this application, the relevant physical time scale is the rate at which environment conditions change, which is much slower. Hence substantial time could be available for computation, perhaps using feedback to gradually adjust the potentials to achieve a desired result.

3.2 Active Materials

Active materials employ quantum smart matter to manipulate their lattice structure to customize their mechanical properties. This could also be used to locally adjust the propagation of phonons or the specific heat of the material, as well as to actively adjust the material's mechanical behavior. These abilities would enable the development of active thermal and acoustic isolators. In addition, such behaviors could be employed to manipulate the displacement of a structure under specific disturbance inputs, or to direct the thermal stresses in a material to a desired location, similar to the way in which a photocopier directs paper along a specific path.

We should note that there are several applications that could be accomplished using classical computers for control. For example, a signal might be sent to a portion of the material to change the state of its control on the lattice structure, modifying the stiffness, ductility, and strength of the material as a result. Such control inputs create a material that (at different times) is both stiff and flexible, depending on what properties were required, and where they were required. One important application of such a material is the forming of high strength alloys. In this instance, a high strength alloy could actively be made more ductile for forming, and then actively re-strengthened once in the proper shape. Such an approach provides an elegant solution for the typical difficulty encountered in industrially forming high strength materials such as titanium.

Similar to the previous example, the relative time scales of physical interaction and computational action are important. In this case, the physical interaction occurs only as fast as the actuator bandwidth, while the computational bandwidth is a function of the quantum computers. The relevant time scale in this example is related to the speed at which it would be desirable to adjust the material properties, which is in turn dependent on the specific applications. However, the applications mentioned can generally operate slowly compared to compuational speeds.

3.3 Adjusting Reaction Rates

Active control of chemical reaction rates takes advantage of the fact that for certain chemical reactions, the reaction rate is affected by the presence of specific charged ions. Quantum smart matter (neutrally charged) could be dispersed throughout solutions containing the reactants to actively control the amount of these charged ions that are (locally) present, thus, actively controlling the reaction rate. A more subtle control would use the local electric fields generated by the active devices in a distributed version of controlling reactions through external fields which can also exploit quantum interference [14, 40]. One possible application would be the control of certain enzyme reactions.

Since reaction rates are generally quite rapid, this application would not involve active feedback response during reactions. Rather the control would take place by modifying the conditions for the reactions at a slower time scale, leading to changes in the overall reaction rate or the mix of products. This could be done both through the reduction of critical reaction elements and by using open-loop field changes previously determined to be useful.

3.4 Active Quantum Springs

Actively controlled nonlinear springs could be created by using quantum smart matter to control the bond strength between two (or several) molecules. Active control of molecules has been discussed in [14] for control of molecular motion. Specifically, electric fields could be generated to control the bond strength between two molecules, creating an active spring which might be utilized in quantum machines.

The relevant time scale in this case is dependent on the application of the active spring created. Specifically, any application of such a spring will have a maximum bandwidth that is necessary. As in the active material example, the bandwidth of any particular application will be dependent on the bandwidth of the actuator. As long as the application bandwidth is slow, relative to the computational bandwidth of the quantum computers, there should be no problem in exerting such control.

4 Conclusions

We have described an application of quantum computers to control the behavior of materials. Even fairly small computers, involving only a few bits, may be able to produce useful new behaviors that would otherwise be difficult to fabricate directly. The use of such programmable materials could allow for experiments on the behavior of many possible structures before deciding which few to actually attempt to fabricate. In this way, quantum smart matter could be used as a simulator for different quantum structures. It could also serve as an experimental platform for examining a range of macroscopic quantum effects by introducing programmable correlations in the overall quantum state of the material.

However, quantum computers face serious implementation difficulties of decoherence and error control [27], especially for programs that require many steps. While substantial difficulities remain before such devices can be constructed, there is encouraging progress in the development of the basic components needed for quantum computation [2, 13, 37]. The simple individual programs useful for smart matter may be less susceptible than others proposed for difficult computational problems, but on the other hand any requirement for communication over large distances will increase the difficulty of avoiding undesired coupling to the environment. This provides another reason to favor local, distributed control methods over the use of global controls. Some local communications among the devices may provide an application for proposals to transmit quantum states [5].

We have suggested some possible applications of such capabilities, but it remains to be seen whether the capacity to operate on superpositions provides enough of an improvement over classical computers to justify the difficulty in maintaining coherence. Finally, if the promise of quantum computing is realized to improve combinatorial search, e.g., for factoring [36, 12] or more general cases [11, 22], this capability could also be used to give very complex potentials for the behavior of matter.

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