

Frustrated computation?

P. van Abswoude¹

¹*Zernike Institute for Advanced Materials, Nijenborgh 4, 9747 AG Groningen, The Netherlands*

Quantum computation can be a fruitful solution to make efficiency steps in computational procedures.

However, the practical arrangements of those systems are still very primitive, and the theoretical possibilities are not really used yet. One of the main problems is the fact that non-unitary decoherence takes place in most single-electron realizations of quantum computation leading to a loss of information. The suggestion of using quantum critical states in the neighborhood of quantum phase transition is discussed and the possibilities to use geometrically frustrated magnetic systems for the practical realization of this are explored in this paper.

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1. Introduction

According to Moore's law [1], the number of transistors in an integrated circuit doubles every two years. This law has been extended to other statements on the development of computer hardware like computational speeds over the past decades. However, due to quantum size effects, these developments cannot continue indefinitely.

One of the concepts introduced to improve computational speeds is quantum computation [2–3]. This is a fundamental different way of computing, compared to the computational principles of classical computers. Instead of classical bits – carrying either the value 1 or the value 0 – qubits are the key elements in quantum computation. These qubits are not 1 or 0, but are in a quantum superposition of those two basis states. This entanglement makes it possible to carry out a series of computations in parallel, fundamentally increasing the efficiency of computers. For example, factorization of a large integer can take polynomially increasing computation times with the famous Shor's quantum algorithm whereas it takes exponentially increasing times in classical algorithms [4–6].

However, the question if quantum computers will ever be in general use is still under debate. One of the most important reasons for this is the decoherence of the entangled electron states that are used in practical realizations of the quantum

computer [7]. This decoherence leads to loss of information stored in the qubits in use. This major problem can be overcome by using superpositions of quantum phases around quantum critical points, as suggested by Sachdev [8].

This paper discusses the possibilities and problems of quantum computation followed by a general introduction into quantum phase transitions and how the therewith associated quantum critical phases can serve as a platform for quantum computation. In the end the aim of this paper is to suggest the use of quantum critical phases in geometrically frustrated magnetic systems for quantum computation.

2. Quantum computing using quantum entanglement

A very interesting fact in quantum mechanics is the occurrence of linear superposition of quantum states. When we have certain eigenstates of a system, any linear combination of these eigenstates is again a solution of the Schrödinger equation.

A physically important example of this is found the valence bound electron pair, which is a superposition of one electron having spin up and the other one spin down on one hand and the opposite on the other hand:

$$\frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

Since both terms in this state are by itself solutions to the Schrödinger equation of the two spin system, all superpositions of those states with the squares of the coefficients adding up to unity, are also solutions.

Based on this situation of superposition, Einstein, Podolsky and Rosen came up with the non-intuitive idea that this can lead to the situation that information is transferred faster than the limit of the speed of light [9]. This possibility is based on

the fact that in the abovementioned state, the electrons are entangled, i.e. their respective states are not anymore independent of the state of the other. Because $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are the measurable states of the system, measuring of the spin state of one of the two electrons leads to a collapse of the wave function of the two electron system and dictates the outcome of the measurement of the spin state of the other electron; irrespective of the location of that electron. This is also called the non-local nature of quantum mechanics. Applications of this concept can be found in e.g. quantum encryption and communication [10–11].

An application of quantum superposition which is less developed in experimental settings is quantum computation. In a classical computer, calculations are carried out on bits that are in a certain state (0 or 1). However, in a quantum computer, qubits (for quantum bit) take the place of bits. Those quantum bits are not in a certain basis state, but in a quantum superposition of those states. Therefore, infinitely many possible states are represented by one single qubit. Several calculations can be carried out in parallel, using quantum entanglement. After the algorithmic steps, a collapse of the wave function takes place. Performing this procedure on many identical quantum systems simultaneously gives a distribution over the possible outcomes from which the coefficients of the actual wave function after application of the algorithm can be deduced. From the change of the coefficients with respect to the original state of the system, a lot more information can be deduced than from calculations on classical bits.

An algorithm of much interest is Shor's algorithm to factorize integers [4]. In classical computers, the times needed for this factorization increases exponentially with the number size. Shor's algorithm allows the factorization with only polynomial increase of the computational time. In this algorithm, only the most crucial step in the factorization process is done by quantum computation. From the distribution of the outcomes of the measurements, the prime factors can be calculated.

The experimental realizations of quantum computational systems are mostly based on solid state systems in which the state is effectively that of single electrons. An example of such a realization is a quantum dot [12]. In this experimental setup, the spin of the excess electron

in a quantum dot is the information carrier of the qubit. Loss and Di Vincenzo proposed detailed suggestions for the realization of quantum gates in such systems [12].

An important characteristic of those systems is that they rely on the coherence of the states of single electrons. However, typical coherence times are often of the same order of magnitude as the clock times of the calculations that are performed and therefore this decoherence introduces errors in the calculations that are not acceptable. The decoherence processes are non-reproducible and information carried in the system is lost. A solution for this problem is proposed by Subir Sachdev [8]. This solution is based on the use of systems that are in quantum critical states.

3. Quantum phase transitions

A classical phase transition occurs when the free energy of a system changes not-analytically [13]. A well-known example is the phase diagram of water showing lines in p,T -space at which the transitions between the solid, liquid and gaseous phases take place; for example the boiling temperature of water is pressure-dependent. A classical critical point is the point after which the phases are no longer distinguishable; above the critical point of water, the densities of the liquid and gas are the same. Also changes in magnetic behavior of solids are classical phase transitions. Phase transitions are the consequence of a versatile interplay between the two components of the free energy: enthalpy and entropy. As a consequence of this, non-zero changes of the entropy are needed and classical phase transitions cannot happen at zero temperature. However, some quantum systems can have non-zero entropy at zero temperature and in those cases we have quantum phase transitions [14].

An example of a quantum phase transition Sachdev comes up with, is that of a square lattice with bosons, with a occupancy $f=1$ [8]. That means that for every site in the lattice, there is exactly one boson. This systems can be in two phases at zero temperature. One is the superfluid state in which the bosons are randomly distributed over the lattice sites. The other phase – which occurs when a potential is applied – is an insulating state in which all lattice points have an occupancy of exactly one boson. Both states

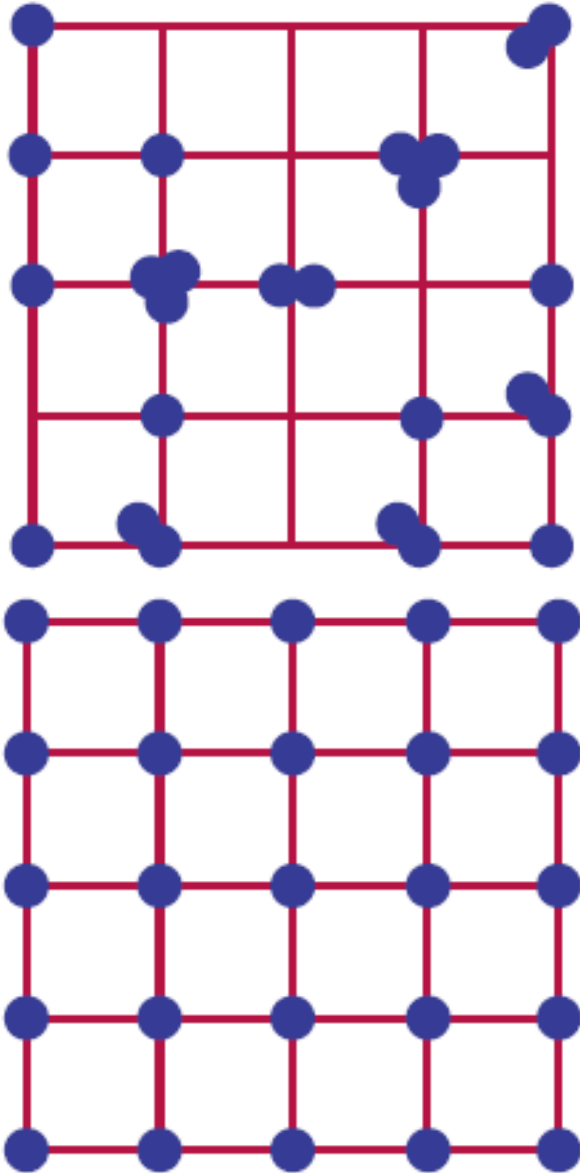


Figure 1: System of bosons in a square lattice in the superfluid phase (top) and the insulating phase (bottom); reprinted from [9].

mentioned are depicted in Figure 1. Since the superfluid phase has a fundamentally higher conductivity than the insulating state, measurement of the conductivity is a good measurement for the phase of the system.

The quantum phase transition takes place at a certain quantum critical point $g=g_c$. As can be understood from the discussion, this g_c occurs at zero temperature. When a finite temperature is added to the system, a so-called quantum critical phase occurs in which the tuning parameter has to differ substantially from the critical value in order to have the system ultimately in one of the two phases, as can be seen in the phase diagram in

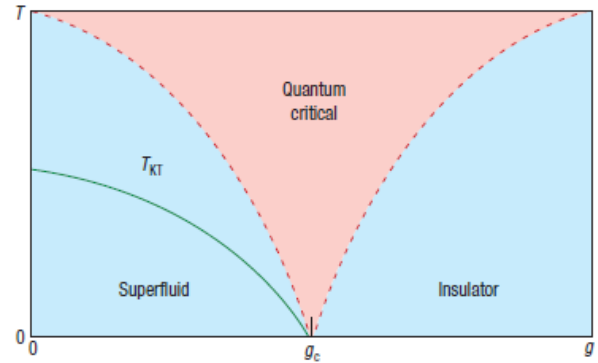


Figure 2: Phase diagram of the boson on square lattice; reprinted from [9].

Figure 2. The quantum critical region is cut off on the upper part of the phase diagram when temperatures are reached for which kT is larger than the energies which are responsible for the different phases [15]. Experimental evidence of the existence of such a quantum critical phase appearing in YbRh_2Si_2 can be found in [16].

Sachdev suggests that those systems of entangled quantum phases in quantum critical phases can be used to make quantum computers possible. The read-out of such systems can be done by measuring certain characteristic transport properties of the system, for example the electrical conductivity of the boson system described above. The measurement should take place after the computational manipulations are carried out on the state. However, this arrangement is not realized to date.

4. Geometrically frustrated magnetic systems

One class of materials exhibiting quantum phase transitions are those with geometrical magnetic frustration. There are a lot of materials showing ferromagnetic or antiferromagnetic behavior; corresponding to their tendency to have a parallel respectively antiparallel alignment of the unpaired electron spins of their atoms. However, when we consider the case of antiferromagnetic behavior in a lattice in which there are three spins interacting and we only consider nearest neighbor interaction, when the first two spins are aligned antiferromagnetically, the third spin cannot “choose” with which it should align and the phenomenon of *geometrical frustration* comes into sight [17–18]. See Figure 3. The same occurs in three dimensions when considering a tetrahedral structure in which all the spins interact antiferromagnetically.

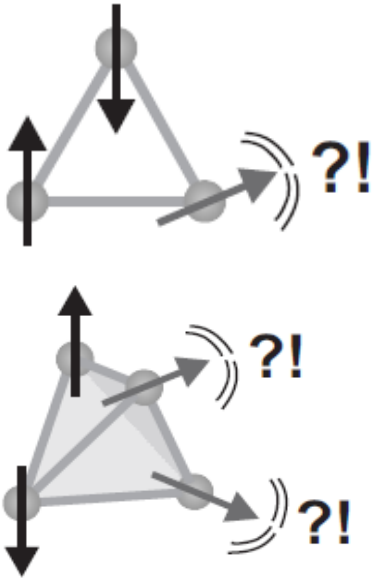


Figure 3. Geometric frustration in a 2D triangular lattice (top) and a 3D tetrahedron (bottom); reprinted from [17].

The most common way of realizing a material with geometrical frustration, are the so-called pyrochlores which are materials with the general formula ABO_3 or $A_2B_2O_7$ in which the A and B ions both have tetragonal sublattices, so they show frustration when A or B is antiferromagnetic. Among this class of materials we find a lot of different properties like ferroelectricity, superconductivity and spin ices and spin glasses [19]. Those systems are called spin-ices because they resemble the entropy-inducing geometry of water ice crystals at zero temperature.

Another common realization of geometric frustration occurs in systems where effective layers of antiferromagnetic centers appear. A nice example is the stacked material $CuFeO_2$ with triangular 2D lattices of magnetically interacting Fe^{3+} ions separated by Cu/O layers [17]. This system is depicted in Figure 4.

The consequence of geometrical frustration in magnetic systems is that there is not a single ground state, but the ground state is macroscopically degenerate. This statement implies that such a system always has a non-zero entropy; even at zero temperature, which is classically in contradiction with the third law of thermodynamics. Therefore quantum phase transitions are expected to be observed between a variety of interesting peculiar phases in geometrically frustrated magnetic systems.

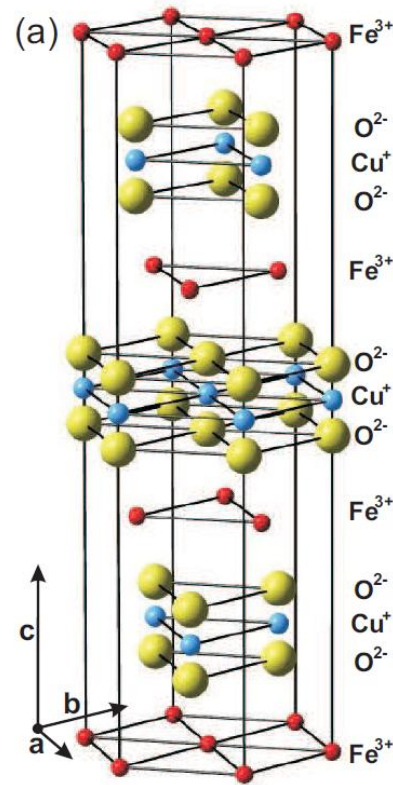


Figure 4: $CuFeO_2$, a compound with a triangular 2D lattice of Fe^{3+} ions; reprinted from [17].

5. Geometrical frustration as a possible realization of quantum computers

As was explained in section 3, Sachdev introduced the possibility to use quantum critical phases of systems to make quantum computational systems. These systems are expected to be much more stable and inert with respect to non-unitary decoherence mechanisms. This gives cause to introduce the idea of geometrically frustrated magnetic systems as the platform for the needed quantum critical phases. The advantage of this idea is that the frustrated systems needed for this setup are relatively easily accessible and a lot of research into them is done at the moment. It seems to be worthwhile to put effort in experiments to explore the possibilities mentioned before. However, not too much should be expected in the nearby future from this technique. There is still a lot to learn about the exact properties of the versatile systems showing geometric frustration. An example can be found in [20], where they experimentally found phases of the geometrically frustrated magnetic material Cs_2CuBr_4 that were not expected from theoretical calculations. To control and manipulate those phases is even one step further than understanding them. The next step is to have more fundamental

inside in the physical meaning of the entanglement present in the quantum critical phases and how to manipulate them. Furthermore, the finite temperature which is needed to enter the quantum critical phase, also introduces thermal entropy to the system which can introduce decoherence also in this kind of machines. When these problems are solved, physical realizations of the operating gates should be made. Altogether there is still a lot of research to be done before this very nice principle can lead to a working device.

6. Conclusion

Despite of the theoretical possibilities of quantum computation, the practical implementations of it are not so many to date. An important problem in the realization of quantum computers is decoherence which is due to non-unitary interactions with the environment. Quantum critical phases which occur near quantum critical points could serve as new systems for the realization of quantum computation because those phases can be seen as linear superpositions of phases. The materials in which those quantum critical phases occur, are systems with degenerate ground states at zero temperature; therefore also carrying non-zero entropy at zero temperature. One class of those systems is formed by geometrically frustrated magnetic systems in which antiferromagnetically interacting spins cannot be in the energetically lowest state because of certain geometrical configurations. The use of such systems for quantum computation should be explored more, but a long way is still to go before we have practical working applications.

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