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Introduction to solid-state quantum computation for engineers

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Abstract

This review is an introduction to solid state quantum computation and its applications for engineers with little or no quantum physics background. Some current classical limits of computation are briefly described, and examples of quantum algorithms are presented to show why quantum computation may be a way of overcoming these limitations. In this review, we have focused on one quantum computer proposal, the Kane proposal. It is a solid-state proposal in silicon doped with ^{31}P atoms. However, significant technological advances will be required in smart electronics, nanotechnology and solid state devices if we are to see a useful solid state quantum computer. © 2002 Published by Elsevier Science Ltd.

Keywords: Smart electronics; Smart structures and materials; Solid state quantum computation

1. Introduction

Very few people will dispute that Moore's Law — the rough rule that says the processing power of computers doubles every 18 months — will break down sometime in the future. A rough projected date is somewhere between 2010 and 2020. What then? Will the computer industry hit a barrier and then stop? Nobody knows, but unless our method of computing changes fundamentally, computers will not be able to keep up with the ever increasing demand of computing power. This paper outlines one approach that has received a lot of attention over the past few years, Quantum Computers (QCs).

Section 2 discusses the current problems that classical computers are facing. Traditionally, increasing the computational power is primarily achieved by shrinking the devices smaller and smaller. There are obviously practical limitations to the manufacturing aspects of computers as well as physical and functional limits as to how small these devices can get. For many of these limitations, there are no known solutions yet. There are also fundamental limits to classical computing. These fundamental limits come about from the way we design and operate our computers, and thus, it is widely accepted that there are no classical solutions, practically or theoretically, to these limits.

Section 3 briefly explains a few basic quantum mechanical concepts and how quantum computers can address many of these issues. By exploiting the strange properties of the quantum world, many conventional problems can be solved much more efficiently on a quantum computer. Algorithms employing superposition and entanglement of quantum bits (qubits) have been shown to dramatically speed up many problems, such as Deutsch's problem [1] and Non-deterministic Polynomial (NP) problems such as finding the two prime factors of a particular number [2] — the key to cracking RSA cryptography. Shor's algorithm employs the technique of quantum Fourier transforms. Another application is Grover's search algorithm [3], which square-roots the conventional processing complexity when searching for a particular item in an unsorted database.

In Section 4, we will describe a particular proposal by Kane [4] to realise a quantum computer in silicon. It is widely believed, and with good reason, that quantum computers will ultimately be realised in solid-state. However, there are some very formidable technological challenges that must be overcome before we see a working solid state QC in action; problems involving the building of a QC as well as the operation of the QC.

2. Limitations of classical computation

As devices shrink smaller, not only do they become harder to make, they become increasingly difficult to manufacture precisely. Even small uncertainties can result in large variations in device characteristics. Larger percentage margins will need to be given in designs. More error correction and control logic will also be required.

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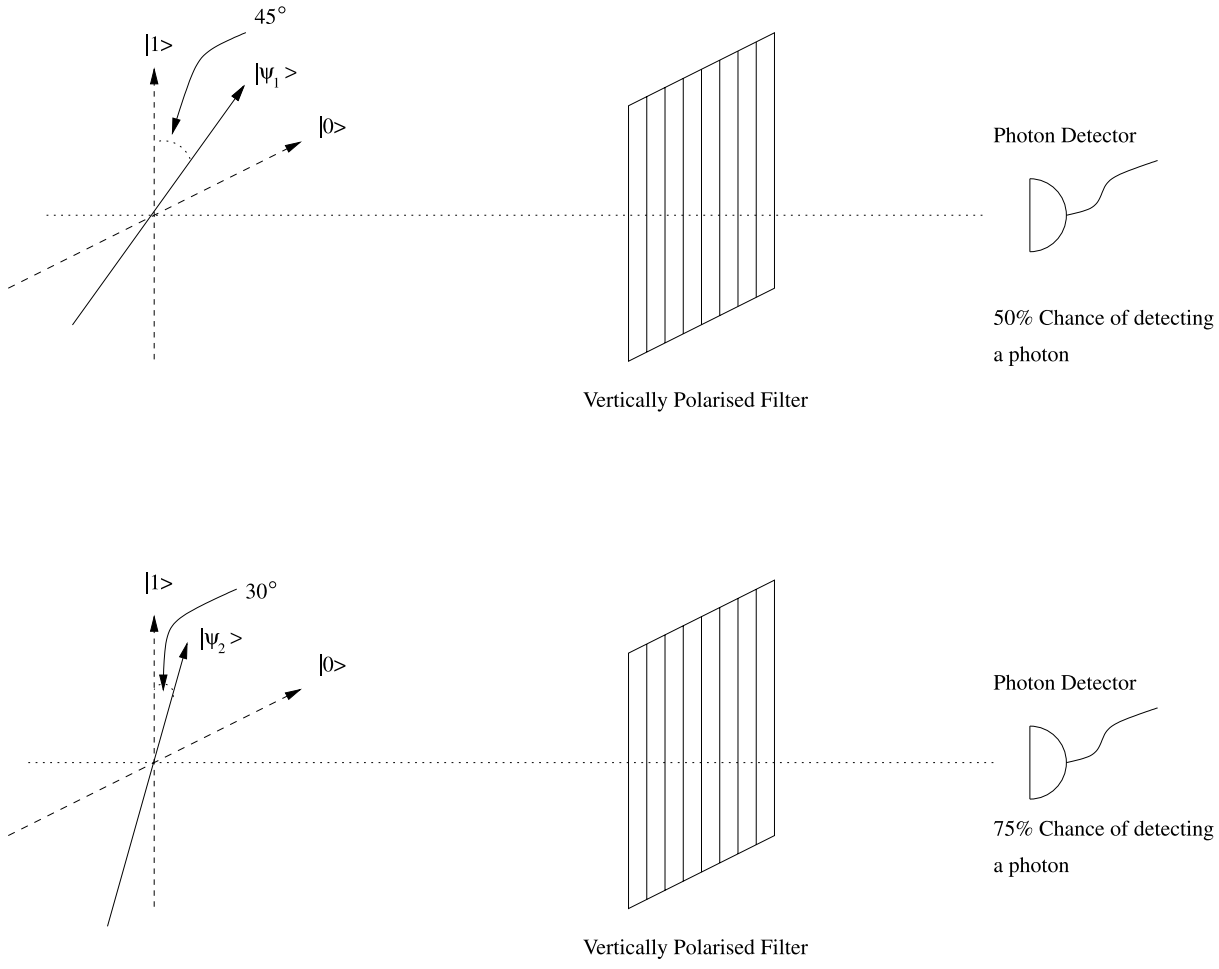

Fig. 1. Using photon polarisation as a qubit. For the 45° polarised photon, the photon detector behind the filter has a 50% chance of detecting that the photon has passed through the filter. For the 30° polarised photon, the chance is increased to 75%.

Classical computers require conducting interconnects to carry the voltage and current signals from one device to another. The capacitances of these wires, is a major limiting factor to the speed in which signals can travel, thus limiting the speed of computation. Much effort has been put into routing interconnects to reduce the length of these wires. As feature sizes continue to decrease, the wires are getting thinner and closer together, thus increasing the capacitance between the wires. Increased capacitance will require more current to maintain the speed of communication. However, the decreased cross-sectional area of the wires places a limit on the maximum current that it can carry.

As more and more circuitry is packed into smaller and smaller areas, the heat generated needs to be removed to avoid destroying the fragile devices. The ability to dissipate power plays a major role in determining the maximum component density of devices. It has been roughly calculated [5] that the maximum gate density using present technology is approximately $1.7 \times 10^7/\text{cm}^2$.

The solubility limit of dopant atoms is also a growing concern when attempting to increase the charge concentration of current devices. As the dopant concentration increases, the dopant atoms interact with each other to form clusters [6]. These clusters increase the impedance of the doped regions, and thus increase the power dissipation of the devices.

Despite all the practical problems of classical computers, there are some fundamental limits of the way we perform computations. In particular, NP problems are inefficient and difficult to solve because the computational resources required, such as time and memory, increase dramatically with the size of the problem. Problems such as factoring of large numbers into its prime factors fall into this category. Quantum computers can help to alleviate some of these problems by reducing the complexity to a polynomial rate of increase rather than an exponential one. However, not all NP problems are expected to be able to be solved in polynomial time by a quantum computer, but since classical computation is a limiting subset of quantum computation, QCs, with appropriate quantum algorithms, will be at least as fast as classical computers adopting classical algorithms.

3. Quantum computers

3.1. Basic quantum mechanics

The power of quantum computation over conventional classical computation comes from the ability to place the 'bits' into a superposition of states and the ability to entangle the bits. These bits are thus called qubits. A qubit has two distinct states, which we can arbitrarily label 0 and 1 for the purpose of computation. These are orthogonal states in Hilbert space. When a qubit is in a superposition, we can think of it as being both 0 and 1 at the same time. However, when we measure the qubit, the superposition will collapse into one of the two states with the probability defined by the nature of the superposition.

The standard notation for expressing these quantum states is the Dirac Bra–Ket notation. Each state is written as $|\psi\rangle$. So, the 0 state is $|0\rangle$, called the 0 ket. A ket is a complex vector in Hilbert space. Superpositions are expressed as vector sums of state kets. In the case of qubits, it is $a|0\rangle + b|1\rangle$, where a and b are, in general, complex probability amplitudes of the respective kets. A measurement is a projection of this superposition onto a set of basis kets, with each of the magnitudes being the probability that we will find the qubit in a particular state. In other words, $|a|^2$ and $|b|^2$ are the probabilities that when we measure the qubit, we will find 0 and 1, respectively. From the conservation of total probability, we can also conclude that $|a|^2 + |b|^2 = 1$.

One of the easiest ways to picture a qubit is by considering photon polarisations (Fig. 1). We can define vertical polarisation of the photon as $|0\rangle$ and horizontal polarisation as $|1\rangle$. Now imagine if we have a single photon of 45° polarisation. What happens when this photon arrives at a vertically polarised filter? This is a measurement of the photon, and thus the superposition will collapse. The photon will collapse into either a vertically polarised or a horizontally polarised state with 50/50 probability. This is an even superposition of $|0\rangle$ and $|1\rangle$, i.e. $1/\sqrt{2}|0\rangle + 1/\sqrt{2}|1\rangle$. Obviously if the photon is vertically polarised, it will pass through, otherwise, it will not. Now if the photon is 30° polarised, then we can see that this is $1/2|0\rangle + \sqrt{3}/2|1\rangle$, and so this means that we have a $|\sqrt{3}/2|^2 = 3/4$ chance of detecting that the photon has passed through the filter.

3.2. Requirements

For any computer, there must be hardware and software. In classical computers, the hardware is the silicon chip, where the bits are represented by different voltages. Classical software forms the higher abstraction level that manipulates the hardware to perform tasks.

In a quantum computer on the other hand, the hardware is the qubits. At the moment, some of the qubits in use could be polarisation of photons (see Section 3.1), physical presence of photons (beam splitters), energy levels of atomic particles [7], the quantum spin of atomic particles [4,8], or recently, the charge states of superconducting materials [9]. In this paper, we will consider Kane's solid state quantum computer proposal, which employs nuclear spins of phosphorous atoms as the qubits.

As with classical software, quantum software need not deal with exactly how the hardware is realised, but rather, what to do with the bits/qubits if and when they are realised. This is where the power of quantum computers becomes apparent. Quantum algorithms such as Shor's factoring algorithm [2], have shown that by exploiting the fuzziness of quantum mechanics we can speed up and solve certain types of problems that classical computer will unlikely be able to solve in a reasonable amount of time.

3.3. Quantum software

This section briefly demonstrates the computational power of a quantum computer. These are not meant to be vigorous derivations of the algorithms, but rather brief descriptions of how they work and the improvements that they provide over classical methods. For detailed mathematical analysis, see Ref. [10].

3.3.1. Deutsch's algorithm

Deutsch's problem [1] is perhaps one of the simplest examples where quantum computers can outperform classical computers. The question is: given $f(x)$ does $f(0) = f(1)$?

Classically, we must calculate $f(0)$ and $f(1)$ then compare the two results. This obviously requires two calculations. Using a quantum network, we can do that in one step (Fig. 2).

What we have in Fig. 2 are three quantum gates that manipulate two qubits. The Hadamard gate, H, puts a qubit in the zero state $|0\rangle$ into an even superposition of zero and one, $|0\rangle + |1\rangle$ (Table 1). While U_f is a unitary controlled-function gate which performs the function $f(x)$ on the second (target) qubit if the first qubit (control) is in the $|1\rangle$ state, otherwise, the gate leaves the qubit alone (Table 2).

At the end of this simple quantum circuit, if we measure the first qubit in the $|1\rangle$ state, then the function is balanced (i.e. $f(0) = f(1)$), otherwise, if it is in the $|0\rangle$ state, then we have an unbalanced function. Despite this simplicity, we can see that we only need to perform the calculation, U_f, just once in the quantum regime, whereas we will need to do it twice classically.

Table 1
Operations of Hadamard gate. For convenience, the normalising constant $1/\sqrt{2}$ is often left out

$\|\psi_0\rangle \rightarrow \|\psi_f\rangle$
$\|0\rangle \rightarrow \|0\rangle + \|1\rangle$ $\|1\rangle \rightarrow \|0\rangle - \|1\rangle$

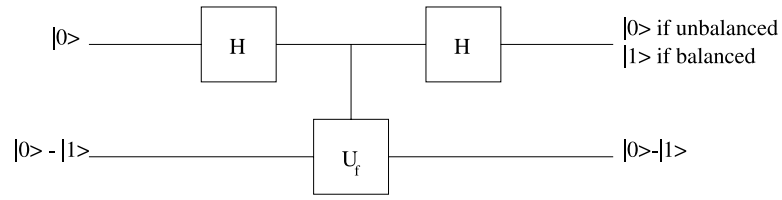

Fig. 2. Quantum circuit for solving Deutsch's problem. The normalising constant $1/\sqrt{2}$ has been left out for convenience.

3.3.2. Quantum fourier transform

Fourier transforms are one of the most important and useful tools in engineering. However, calculating the Fourier transform is not an easy task computationally. Classically, the discrete Fourier transform (as opposed to continuous FT since we are dealing with digital systems) is defined as $y_k = 1/\sqrt{N}\sum_{j=0}^{N-1} x_j\, e^{2\pi ijk/N}$.

A fast and widely used classical algorithm for computing the DFT is the Fast Fourier Transform (FFT), which is of order $O(n2^n)$ (where the number of elements $N = 2^n$).

On the other hand, quantum Fourier transform (QFT), defined as $|a\rangle \rightarrow 1/\sqrt{N}\sum_{b=0}^{N-1} e^{2\pi iab/N}|b\rangle$ can provide significant speedup.[1] So how fast is the speedup?

For computational purposes, the above equation can be written in a more convenient tensor product form,

$$|a_1, a_2, \ldots, a_n\rangle \rightarrow \frac{(|0\rangle + e^{2\pi 0 a_n}|1\rangle) \otimes (|0\rangle + e^{2\pi 0 a_{n-1}a_n}|1\rangle) \otimes \cdots \otimes (|0\rangle + e^{2\pi 0 a_1 a_2 \ldots a_n}|1\rangle}{2^{n/2}}$$

where $0a_1\ldots$ are binary fractions given by $a_1/2 + a_2/4 + \cdots + a_n/2^n$. This leads to the circuit in Fig. 3.

As can be seen in Fig. 3, for 2^n elements, there are $n(n+1)/2$ gates involved in performing a quantum Fourier transform. Thus, the complexity of the QFT circuit is $O(n^2)$ which is polynomial! So by doing the transformation in the quantum regime, we have an exponential speedup over the classical Fourier transform method.

Unfortunately, this method cannot be used to simply replace FFTs in conventional applications. In the QFT, the results are probability amplitudes, which means that we cannot directly measure them. To make use of the QFT, we need applications, which are also in the quantum regime, which makes use of and manipulates quantum probability amplitudes. One such application is Shor's factoring algorithm.

3.3.3. Shor's algorithm

Shor's factoring algorithm [2] is one of the spectacular applications of quantum Fourier transform.

If we know two prime numbers, x and y, then finding the product $N = x \times y$ is easy. However, if we only know N, finding the factors x and y is an NP problem. This difficulty in factoring large numbers is the basis of many public key encryption schemes, such as RSA encryption.

To solve this, given N, the naive method of factoring it into its prime factors is to simply starting from 1, and then working upwards until we have found one of the prime factors, which will give us the second one very easily. This requires $\sqrt{N}$ tries for the worst case scenario.

Without going into too much detail and numerical verification, Shor's algorithm is as follows:

1. Find random co-prime number $a < N$.
2. Compute $f(x) = a^x \bmod(N)$.
3. Find period, r, of $f(x)$, i.e. $f(x + r) = f(x)$.
4. x and y are the greatest common denominators of N and $a^{r/2} \pm 1$.

For example, Let $N = 15$.

1. Choose $a = 7$.[2]
2. Compute $f(x) = 7^x$ then $\bmod(15) = 1, 7, 4, 13, 1, 7, 4, 13, \ldots$.
3. Period, $r = 4$.
4. $x = \mathrm{GCD}(15, 7^{4/2} + 1) = 5$, $y = \mathrm{GCD}(15, 7^{4/2} - 1) = 3$.

The hard part is step 3, finding r. Using the binary form of

Table 2
Operations of a Controlled-Function gate. The simplest example is where $f(x)$ acts as an inverter such that $f(0) = 1$ and $f(1) = 0$. In this case, what we have is an XOR gate. In the quantum computating community, this two qubit XOR gate is known as the Controlled-NOT gate

$\|\psi_0\rangle = \|q_1 q_2\rangle_0 \rightarrow \|\psi_f\rangle = \|q_1 q_2\rangle_f$
$\|0\rangle\|0\rangle \rightarrow \|0\rangle\|0\rangle$
$\|0\rangle\|1\rangle \rightarrow \|0\rangle\|1\rangle$
$\|1\rangle\|0\rangle \rightarrow \|1\rangle\|f(0)\rangle$
$\|1\rangle\|1\rangle \rightarrow \|1\rangle\|f(1)\rangle$

[1] QFT is in fact an example of a more general algorithm; that of Kitaev's phase estimation algorithm. See Ref. [10] for an extensive discussion on QFT and Kitaev's algorithm.

[2] Although $a = 14$ also satisfies the condition that a is a co-prime of N, the reader may notice that the algorithm does not produce the correct result. Shor's algorithm is a probabilistic algorithm, which is not a major issue as failure is easily detectable. For large N, the chance of finding an a that works is very high. For $N = 15$, any of 2, 4, 7, 8, 11 or 13 would work.

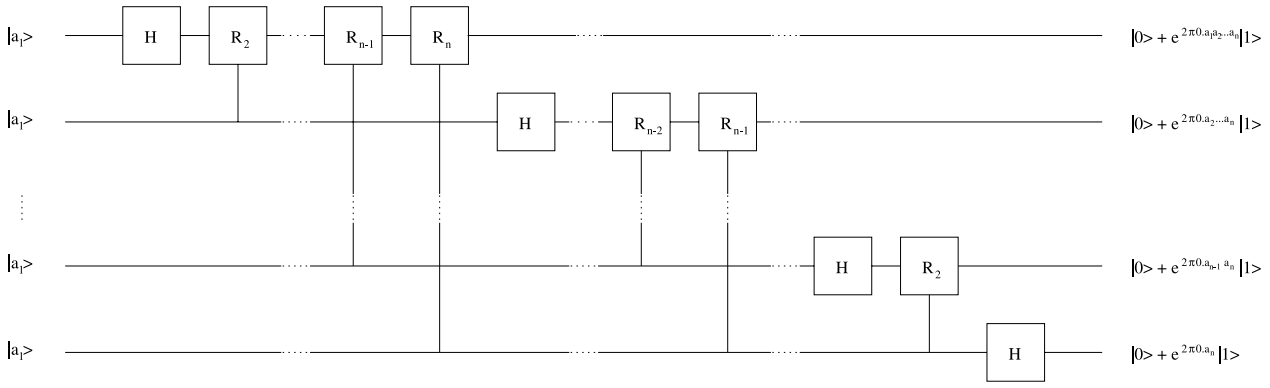

Fig. 3. QFT quantum circuit representation. The H gates are the Hadamard gates, while the R_n gates are Controlled-Function gates that perform $e^{2\pi i/2^n}$ if both the control and target qubits are in the $|1\rangle$ state.

$N = 2^n$. It is an order-finding problem of complexity $O(N) = O(2^n)$. However, through application of quantum Fourier transforms, we can speed up this difficult step exponentially.

1. We start off with initial state $|0\rangle|0\rangle$.
2. Create the superposition $1/\sqrt{2^t}\sum_{x=0}^{2^t-1}|x\rangle|0\rangle$.
3. Apply an unitary operator such that $|0\rangle \rightarrow |f(x)\rangle$ resulting in $1/\sqrt{2^t}\sum_{x=0}^{2^t-1}|x\rangle|f(x)\rangle$.
4. Apply QFT to $|f(x)\rangle$ resulting in

$$\frac{1}{\sqrt{2^t}\sqrt{r}}\sum_{x=0}^{2^t-1}|x\rangle\sum_{l=0}^{r-1}e^{2\pi i l x/r}|F(l)\rangle.$$

5. Apply inverse QFT to the first quantum register, $|x\rangle$, resulting in $1/\sqrt{r}\sum_{l=0}^{r-1}|l/r\rangle|F(l)\rangle$.
6. Measure $|l/r\rangle$ to get l/r.
7. Obtain r.

Steps 4 and 5 are both $O(n^2)$ so factoring has become a polynomial increase problem!

Now, our initial choice of a is very important, and it is easy to see that not all a values give the right result. This is not a major issue, since verification is very easy. For factoring large numbers, this method will find x and y with a probability very close to 1.

3.3.4. Grover's algorithm

Grover's algorithm [3] provides a less significant speed up to the everyday problem of searching an unsorted database than Shor's algorithm did to factoring large numbers. However, the fact that there is still an improvement demonstrates that quantum computers are not limited to simply one class of problems.

The problem we have here is simple. Given an unsorted database, how are we to find a particular item that we want? On a classical computer, a method to perform this search is to start from the beginning and check each element one at a time. For $N = 2^n$ elements, this obviously has complexity $O(2^n)$. Grover's quantum search algorithm reduces this complexity to $O(\sqrt{2^n})$. This is only a quadratic improvement, but is an improvement nonetheless. Grover's algorithm assumes that there is only one correct item in the database. Other techniques have evolved from this base to count the number of correct items in the database [11] and finding matches between two databases [12].

4. Quantum hardware: Kane's solid state computer

Section 3.3.4 demonstrated that quantum computers can significantly improve the efficiency of real-life problems. This section describes one proposal of realising a quantum computer. Ref. [13] gives descriptions of other solid state QC proposals.

4.1. How does it work?

The Kane proposal [4,14,15] is a silicon based solid state computer. The qubits are nuclear spins of phosphorus (^{31}P) donor atoms embedded in the silicon lattice (Fig. 4). ^{31}P was chosen because it is very well isolated from the environment with electron relaxation time of thousands of seconds and nuclear spin relaxation times of greater than 10 h at low temperatures. It is estimated that phonon limited spin relaxation time is of the order of 10^{18} s in the milliKelvin range [16]. Also, ^{31}P being approximately the same size as a silicon atom, can readily replace a silicon atom in the lattice. For a detailed analysis of the physics in the Kane propsal, see Ref. [15].

^{31}P atoms have five valence electrons. With four of these electrons involved in covalent bonds with the neighbouring silicon atoms, at low temperatures, it has effectively one bound electron like a hydrogen atom. However, for ^{31}P atoms, there is a two fold electron spin degeneracy at the ground state, and so, using perturbation theory, an external magnetic field, B, needs to be applied to break this degeneracy. The phosphorus nuclear spins are coupled to their electron spins by the hyperfine interaction. The A-Gates above the donor atoms control the strength of the hyperfine

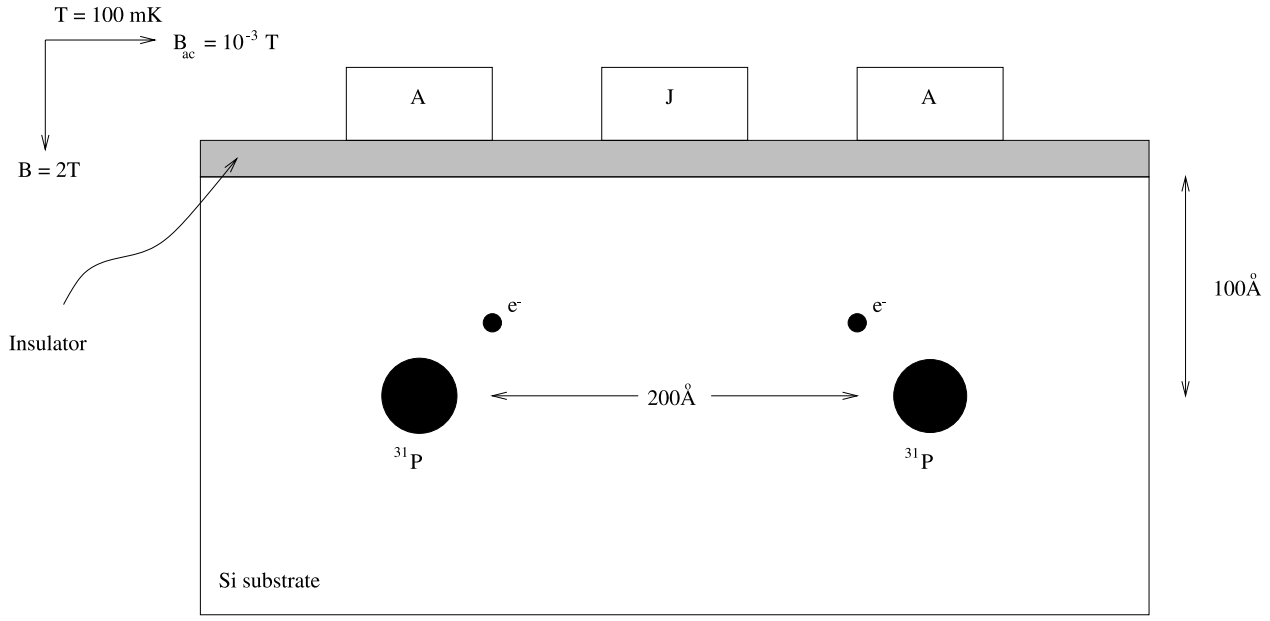

Fig. 4. Schematic of Kane's solid state Si:P quantum computer.

interaction, which alters the resonant frequency of the ^{31}P nucleus. This system is a voltage-controlled oscillator. When a positive voltage is applied, it shifts the electron wave function away from the ^{31}P nucleus towards the gate, thus lowering the resonant frequency (Fig. 5). Now by applying a global AC magnetic field, B_{ac}, we can arbitrarily rotate the nuclear spin at resonance. Two qubit operations are performed by turning the electron-mediated coupling between two donor atoms on and off using the J-gates positioned between the A-gates (Fig. 6).

One proposal for nuclear spin readouts is done by applying different voltages on the A-gates and detecting the resulting electron movement [4]. Pauli exclusion principle dictates that only electrons with opposite spins can occupy the same orbital space, and thus if the electrons are indeed in opposite spins, there should be a detectable electron current from the donor under the negatively biased gate to the positively biased gate. Single Electron Transistors (SET) have been proposed to detect this electron current [17]. The minimum error rate due to external noise for this proposal is of the order of 10^{-6} per second for typical values of noise [18].

4.2. Technical difficulties

So far, we have avoided discussing the practical difficulties in realising the above proposal. The technological challenges involved are currently beyond our capabilities today, but not inconceivably so.

First of all, the silicon host needs to consist of almost completely pure spin zero, charge neutral isotopes. Secondly, the entire slab of Si:P needs to be cooled to the milliKelvin range during operation. This is generally done in a dilution fridge. At high temperatures, the electron and nuclear spins have too many degrees of freedom. We need to

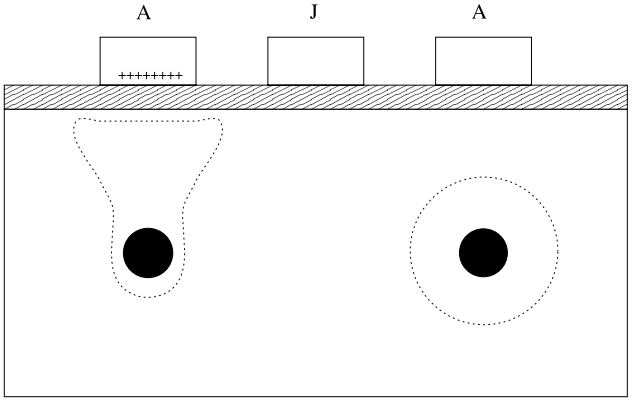

Fig. 5. When a positive bias is applied to the A-Gate, the electron cloud is attracted towards the gate, thereby lowering the resonant frequency of the nucleus.

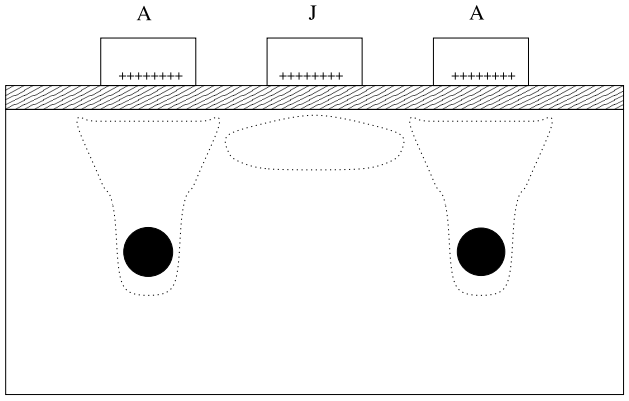

Fig. 6. Neighbouring nuclei are coupled by applying a positive bias to the J-Gate.

reduce phonon-induced decoherence as much as possible. Also, at high temperatures, the electrons will generally not remain bound to their donor nuclei to participate in the electron–nucleus coupling.

The most difficult technological hurdle, however, is in fabrication. The phosphorus donors must be placed in an ordered array, with exactly one donor per array cell. Neighbouring donors are required to be far enough apart so that, under unbiased conditions, their electron wave functions do not overlap, while still close enough for strong coupling between the nuclei during operation. These conditions limit the separations to be approximately 100–200 Å [4,15]. Atom-optics and ultra-high-vacuum scanning tunnelling microscopy are being investigated as possible methods for creating the donor array [4]. After the donors have been placed, the next task is to then bury the donor arrays in more pure silicon. The current practice is to grow the silicon at temperatures of around 600 K, which is unsuitable, considering the donors were placed onto the silicon at 4 K before hand. The high temperature will cause too much movement of the ^{31}P atoms. Once the silicon is somehow grown and the oxide layer has been deposited, the donors will then have to be found again. It has been proposed that a scanned probe with a SET at the tip could be used to locate the hidden donor [17], a bit like a 'metal' detector. However, the $-e$ electronic signal due to the extra electron could be too weak to be detected under a few hundred Angstroms of silicon, since there is a $+$e nucleus nearby. After the donors have been located, the A-Gates must be constructed directly above the donor nuclei, while still managing to fit a J-Gate between them. Thus, the minimum feature size for the construction of the gate should be no more than 0.1 μm. This is on the border of the current state-of-the-art technology.

4.3. Future prospects

The Kane proposal has many advantages over other proposals. It is expected to be more readily scalable to large number of qubits and its rate of decoherence should be slow enough to allow error correction techniques to be used. As a working model is yet to be constructed, we are yet to verify whether these expectations are indeed valid.

Fabrication technological challenges aside, it can thus be considered a second generation quantum 'computer'. It is one that can be used to demonstrate and experiment with more advanced quantum computing methods and algorithms.

Acknowledgements

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