## Helical Logic

by
Ralph C. Merkle
Xerox PARC
3333 Coyote Hill Road
Palo Alto, CA 94304
merkle@xerox.com
http://merkle.com/merkle
and
K. Eric Drexler

Institute for Molecular Manufacturing
123 Fremont Avenue
Los Altos, CA 94022
http://www.foresight.org/Drexler.html
This article has been accepted for publication in Nanotechnology. Further information about Nanotechnology is available from URL "http://www.zyvex.com/nanotech/IOP.html"

This article is available from URL "http://www.zyvex.com/nanotech/helical.pdf"
Copyright 1992 by Xerox Corporation and the Institute for Molecular Manufacturing. All Rights Reserved.


#### Abstract

Helical logic is a theoretical proposal for a future computing technology using the presence or absence of individual electrons (or holes) to encode 1 s and 0 s . The electrons are constrained to move along helical paths, driven by a rotating electric field in which the entire circuit is immersed. The electric field remains roughly orthogonal to the major axis of the helix and confines each charge carrier to a fraction of a turn of a single helical loop, moving it like water in an Archimedean screw. Each loop could in principle hold an independent carrier, permitting high information density. One computationally universal logic operation involves two helices, one of which splits into two "descendant" helices. At the point of divergence, differences in the electrostatic potential resulting from the presence or absence of a carrier in the adjacent helix controls the direction taken by a carrier in the splitting helix. The reverse of this sequence can be used to merge two initially distinct helical paths into a single outgoing helical path without forcing a dissipative transition. Because these operations are both logically and thermodynamically reversible, energy dissipation can be reduced to extremely low levels. This is the first proposal known to the authors that combines thermodynamic reversibility with the use of single charge carriers. It is important to note that this proposal permits a single electron to switch another single electron, and does not require that many electrons be used to switch one electron. The energy dissipated per logic operation can likely


be reduced to less than $10^{27}$ joules at a temperature of 1 Kelvin and a speed of 10 gigahertz, though further analysis is required to confirm this. Irreversible operations, when required, can be easily implemented and should have a dissipation approaching the fundamental limit of $\ln 2 \mathrm{x} k T$.

## Introduction

Trends in computer hardware are leading toward higher density and lower energy dissipation. Ultimately, some approaches should result in packing densities in excess of $10^{7} \operatorname{logic}$ devices in a cubic centimeter(Carter et al. 1988, Drexler 1992) (although the current proposal might require a somewhat larger volume). The trend towards higher packing density strongly influences energy dissipation. Conventional devices must dissipate more than $\ln (2) \times k T$ joules in switching; so $10^{17}$ conventional devices operating at room temperature $\left(\ln (2) \times \quad k T \sim 3 \times 10^{-21}\right.$ joules for $T=300$ Kelvins) at a frequency of 10 gigahertz would dissipate $>3,000,000$ watts; a computer with 1,000 times as many logic elements would still be of reasonable size but would dissipate $3,000,000,000$ watts.

Conventional circuits perform more poorly. Even an idealized device which used a one volt power supply and dissipatively discharged a single electron to ground during a switching operation would dissipate one electron volt per switching operation. At $T=300$ Kelvins, this is $40 \mathrm{x} k T$ per switching operation or about $160,000,000$ watts for a computer with $1 \theta^{20}$ logic elements operating at 10 gigahertz. If each switching operation involves hundreds of electrons then energy dissipation enters the multigigawatt range.

New thermodynamically reversible circuits (including CMOS, nMOS and CCD-based logic circuits(Hall 1992, Merkle 1993c, Younis and Knight 1993, Koller and Athas 1992, Merkle 1992)) would fare better, but these circuits still have dissipative losses caused by the resistance of the circuit. While resistance in sufficiently small wires can be very low(Sakaki 1980), if such wires are connected to each other, to logic elements or to larger structures it is common to find resistances of the order of $13 \mathrm{~K} \Omega$ (half of $\mathrm{h} / e^{2}$, where h is Planck's constant) (note that no claim is made that the successful operation of such circuits must fundamentally require resistances of this magnitude, we simply note that shrinking current circuits to a small scale would result in such resistances: further research in this area might be successful in dealing with this problem). Assuming that 100 electrons were required to charge and discharge the wires and capacitive loads in each logic element, and assuming a resistance of approximately $13 \mathrm{~K} \Omega$, we would still find our $1{ }^{20}$ gate computer dissipating over 50 megawatts even using these particular thermodynamically reversible methods.

If the exponential trends of recent decades continue, energy dissipation per logic operation will reach $k T$ (for $T=300$ Kelvins) early in the next century(Landauer 1988). Either energy dissipation per logic operation will be reduced significantly below $3 \times 10^{-21}$ joules, or we will fail to achieve computers that simultaneously combine high packing densities with gigahertz or higher speeds of operation. There are only two ways that energy dissipation can be reduced below $3 \times 10^{21}$ joules: by operating at temperatures below room temperature (thus reducing $k T$ ), or by using thermodynamically reversible logic. Low temperature operation doesn't actually reduce total energy dissipation, it just shifts it from computation to refrigeration (Halliday and Resnick 1988). Thermodynamically reversible logic elements, in contrast, can reduce total energy dissipation per logic op-
eration to $\ll k T$. This paper analyzes a proposed thermodynamically reversible single electron logic system. To achieve high reliability while switching single electrons, we analyze operation at $\sim 1$ Kelvin.

## Reversible Architectures and Logic Proposals

One concern about this approach is the need to use reversible computer architectures. Such architectures are entirely feasible(Landauer 1988, Fredkin and Wffoli 1982, Bennett 1982, Bennett 1988, Bennett 1989, Merkle 1993b, Ressler 1981, Hall 1992, Fredkin and Dffoli 1978, Seitz et al. 1985, Merkle 1993c, Landauer 1961, Landauer 1981, Bennett 1973, Bunis and Knight 1993) and will not be discussed further here. Bennett(Bennett 1989) has proposed very general methods for converting arbitrary irreversible computations into time and space efficient $r$ versible computations.

A wide variety of reversible device proposals have been made(Drexler 1988, Likharev 1982, Likharev et al. 1985, Drexler 1992, Fredkin and Toffoli 1978, Seitz et al. 1985, Merkle 1993c, bunis and Knight 1993, Koller and Athas 1992, Merkle 1992). The present proposal is abstractly similar to billiard ball logic(Bennett 1985, Fredkin and कffoli 1982), and in particular uses the concept of a "switch gate" or "interaction gate."

In billiard ball logic(Fredkin and Toffoli 1982), a set of billiard balls are fired into a set o immovable reflectors at a $f$ ed speed. As the billiard balls bounce of each other and off the reflec tors, they perform a reversible computation. Provided that the collisions between the billiard balls and between the billiard balls and the reflectors are perfectly elastic, the computation can procee at a fi ed finite speed with no ene gy loss.

As originally proposed, this "ballistic" model of computation suffers from the shortcoming that the positions of the reflectors and the initial elocity of the billiard balls must be perfectly accurate. In the real world, the computation would rapidly deteriorate into chaos unless some restoring force maintained the alignment of the billiard balls. Landauer(Landauer 1981) proposed exactly this, suggesting that the billiard balls should remain in the trough of a moving periodic potential (illustrated in Figure 4).

Billiard ball logic is usually thought of in connection with Fredkin gates(Fredkin and Toffoli 1982). Fredkin gates are conservative three-input three-output gates that are logically complete, e.g., any computation can be implemented by an appropriately connected set of Fredkin gates. An appropriately arranged set of reflectors can be used to implement a Fredkinate from billiard balls. Rather than considering the Fredkin gate we will focus instead on the switch gate(Fredkin and đffoli 1982). This can be used to make a Fredkin gate (and so is also logically universal) but it is physically simpler and easier to implement.

A Fredkin gate is illustrated in Figure 1, a switch gate is illustrated in Figure 2, a method of implementing a Fredkin gate from switch gates is shown in figure 3, while a billiard ball being car ried along by a periodic potential is shown in Figure 4.

While the abstract concept of billiard ball logic has been knwn for some time, the idea of implementing this approach by replacing the billiard balls with char ged particles is surprisingly recent(Merkle 1993c) (though Landauer(Landauer 1981) did refer to an unspecified short rang repulsion). In the present proposal, we replace the billiard ball with a single electron. While other


Figure 1.
A Fredkin Gate
charged particles or charged packets of particles can be used, we will focus on the single electron implementation because of the obvious long term performance advantages. The concept that future electronic devices might use single electrons is becoming more accepted(Likhare vand Claeson 1992, Washburn 1992, Grabert and Devoret 1992). This is the first description of a thermodynam ically reversible switching device using single electrons. Not only are we switching single electrons, we are also using single electrons to control the switching (unlik e many proposals which require many electrons to switch a single electron). It is plausible that thermodynamically reversible single electron switching devices will be the ultimate evolutionary end point of electronic logic devices. The authors emphasize that other proposals for single electron thermodynamically reersible logic devices will certainly be advanced, so the present proposal must be viewed as the first $i$ a class rather than "the" one and only design for a single electron thermodynamically re versible logic device.


Figure 3.


Implementation of a
Fredkin Gate
from Switch Gates
(after Fredkin and Toffoli 1982)

While the analysis here focuses on the case of a "charge packet" consisting of a single electron, the use of a multi-electron char ge packet would clearly be simpler in terms of a more near term implementation. In particular, charge packets are commonly used in CCD's. By making a series of design choices in favor of near term feasibility we can arri ve at a design which is basically a thermodynamically reversible type of CCD logic. This possibility is discussed more fully in (Merkle 1993c). The performance of such a system would likely fall well short of ultimate limits for pragmatic reasons. The present paper focuses on an approach which should be feasible in the long term (though less lik ely to be practical in the near term) and which of fers the possibility of


Figure 2.
Schematic diagram of a switch gate

## Billiard Ball



Periodic Moving Potential
Figure 4
Billiard ball being carried along
by a moving potential
greatly superior performance and, in particular the possibility of very low energy dissipation while still operating in the gigahertz range or higher.

## Clock Distribution using Rotating Electric Fields

The periodic moving potential (illustrated in figure 4) which dr ves the electrons forwards can be viewed as a periodic clock signal. It is conentional in today's circuits to distribute clock signals using wires. This approach is energetically disadvantageous because the propogation of the clock signal through wires is itself dissipative, as well as requiring a complex (and space consuming) network for distribution. An attractive alternative is to use time varying electric fields. e propose the use of rotating electric fields as these are conceptually simple, easy to produce, and adequat to drive a wide range of logic devices.

The picture of clock distribution being proposed here is new (though it is abstractly similar to the rotating magnetic field used to clock and p wer magnetic bubble devices(Bobeck and Scovil 1971, Kinoshita et al. 1976)). The computing element is immersed in a rotating electric field. Th electric field, and hence the clock, is vailable at every point in the device and yet no wires are required to distribute it. This reduces energy dissipation and eliminates the space that would otherwise be occupied by the clock distribution network.

A rotating electric field is rather di ferent from a periodic moving potential. In order to achieve the same effect (e.g., to move electrons forwards along their path) we propose the use of helical paths, with the electric field rotating at right angles to the axis of the path. The electron will b confined to part of a single turn of the helix and as the electric field rotates the electron will moved along the helical path much as water is moved along an Archimedes screw. This is illustrated in figure 5

If we were to examine the potential at any point along the helical path we wuld find that it aried in a sinusoidal fashion much as the potential varies along a straight path under the influence of


Figure 5.
Electron being carried along a helical path by a rotating electric fiel
moving periodic potential. The use of a periodic moing potential with straight paths (as shown in figure 4) and the use of a simple rotating electric field with helical paths produce ery similar results. In either case, the electron is moved along the path.

There are other methods of providing a moving periodic potential that do not ivolve distribution of clock signals through wires. A simple proposal would be to have a circuit on the surface of a rotating disk, with an opposing disk with fi ed charges on it. The relative motion of the two disks would result in a moving potential that would clock the circuit. Alternatively, instead of disks two tubes of differing diameter, one tube placed inside the other, could be used. Circuitry could be placed on the inner surface of the outer tube, while fi ed charges could be placed on the outer surface of the inner tube. Again, relative motion of the inner tube with respect to the outer tube could provide a moving potential. This approach also has the advantage that the tubes could be reduced in radius to a very small size (nanometers) and the rotational speed of the inner tube could be made very high (gigahertz) without any fundamental problems. Many such tubes could be stacked adjacent to each other, and charged particles being swept along a potential on one tube could move to an adjacent tube, provided that the movements of the clocking potentials in the two adjacent tubes were appropriately synchronized. A different approach would be to operate the circuit on a piezomechanical surface in which surface acoustic waves created a moving electric potential.

We will not consider the many possible alternatives in this paper.

## The Basic Idea

In helical logic, information is encoded in the presence or absence of indwidual electrons. Electrons are moved from place to place along helical paths. When two helical paths are brought into close proximity the electrons interact through electrostatic repulsion, thus producing an electronic switch gate. The electronic switch gate involves two incoming and three outgoing helical paths. One incoming helical path is termed the "data" path while the other is termed the "condition" path. The two descendants of the data path are called simply the "left" and "right" paths. The electron in the data path will be steered to either the left or right path depending on the presence or absence of an electron in the condition path. This is illustrated schematically in figure 6

The reverse of this operation, in which three incoming helical paths produce two outgoing helical paths, is similar but "run backwards" in time. Because the basic operation of a switch gate is reversible, it can be operated in either the forwards or reverse direction. We will therefore not explicitly analyze this process. Note that in reverse operation it is essential that the presence or absence of a charge carrier on the data path be correctly correlated with the path (left or right) along which the switched charge is entering the switch gate. This constraint can be met (as illustrated in figure 3 showing the design of the Fredkin gate).

It is worth noting that irreversible operations are sometimes convenient. A basic irreversible operation in helical logic merges two incoming helical paths into one outgoing helical path (and dispenses with the data path). Such an irreversible logic operation, if properly designed, should have an energy dissipation which approaches the fundamental limit: $\ln 2 k T$. Helical logic has the valuable ability to degrade gracefully when irreversible operations are required.

We will focus primarily on fundamental issues of device performance while neglecting the issues involved in manufacturing any specific d vice. Thus, we will simply assume that the ability to economically manufacture atomically precise semiconductor material, with dopant atoms placed at atomically precise lattice coordinates, is available. Such a manufacturing technology is not available today but should be available at some point in the future(Drexler 1992, Merkle 1994). In the long run, if we are to achiee the maximum performance possible from semiconductor deices,

we will have to develop and use some sort of molecular manufacturing technology. This is true almost regardless of the specific details of the d vice proposal. The more precisely a device can be fabricated, the better the achievable performance. The limit of this trend will be devices in which each atom is in the right place.

There are many choices for the materials that comprise the helical path and the surrounding medium. An obvious choice is GaAs and AlAs(Sze 1990). Electrons prefer GaAs to AlAs by about 0.3 ev(Van de Walle 1989), so by operating at a suficiently low temperature complete confinemen of the electrons could be achie ved. Another choice would be Ge and Si(Sze 1990, Bean 1992). Other possibilities that should become feasible in the future with the advent of molecular manufacturing(Drexler 1992, Feynman 1960), would be Si and GaP(Sze 1990), Si and ZnS (Sze 1990), or even C (in the form of diamond) and vacuum. The latter would offer significant advantages because of the low dielectric constant of vaccuum, although the negative electron affinity of the hydrogenated diamond (111) surface suggests that either the use of holes as the charge carriers or the modification of the diamond surface to achieve a positive electron affinity (i.e., fluorinated diamond (111)) would be advantageous. If the helical channels are diamond with hydrogenated diamond (111) surfaces, an electron in the channel would tend to escape into the surrounding vacuum. The idea that a hole might perform a similiar feat is less plausible. Diamond channels with fluorinated surfaces in vaccuum using either electrons or holes (or both) as charge carriers might be an attractive choice once our manufacturing technology is able to build the required structures.

The negative electron affinity of the hydrogenated (111) diamond surface also suggests the use of an evacuated channel surrounded by walls of diamond. This approach means the channels are holes bored in a block of diamond. The motion of electrons through evacuated channels might prove advantageous by reducing electron/channel interactions. The creation of a helical tube with relatively smooth walls in a block of unstrained diamond would require the use of more than just the (111) plane. Fluorinating or otherwise modifying other surfaces (e.g., (100) or (110)) so that they would have negative electron affinity should be feasible, and would permit a tube with smoother walls. Approaches using strained diamond (e.g., diamond which is curved by, for example, the introduction of appropriately placed dislocations (Merkle 1993a)) would be another alternative.

The use of other charge carriers produces a wider range of possibilities. For example, the charge carrier could in principle be a single proton. The channels would then be pores through which $\mathrm{H}^{+}$ could easily move. The increased mass of $\mathrm{H}^{+}$(as compared with an electron) would simplify confinement by decreasing the effective distance through which the charge carrier could tunnel. Channel size and interchannel distances could both be made much smaller; proton-proton repulsive interactions would therefore be larger and operating temperature could be increased. The smaller size and higher operating temperature of a helical logic system based on hydrogen ions would compensate to some extent for the slower speed, and the result might be advantageous in some applications. Many other small ions could also be used.

The use of charge packets made up of many electrons (or holes) should provide a method of implementing helical logic using today's technology at higher temperatures. The use of charge packets is common in CCDs. It is an open question whether today's technology can economically mass produce the complex structures needed for helical logic (though research devices should be feasible). However, a 2D version of helical logic which used spiral paths should be feasible with to-
day's technology. The implementation of a planar switch gate should likewise be feasible. More research on this point would be worthwhile.

Whatever the materials choice and manufacturing technology, the primary requirement is that a charge carrier be confined to a helical path, and be able to interact with other charge carriers in other helical paths.

## Energy Dissipation

Energy dissipation is caused by three main factors: energy loss during charge transport, energy lost to the material in the absence of chage carriers (the dielectric loss factor), and energy loss during switching operations. All three loss mechanisms are a function of clock frequency. We will call these transport loss, dielectric loss and switching loss. Energy loss will also occur when irreversible logic operations occur We will neglect this source of enegy loss in the following analysis, as it will vary widely depending on the logical design of the system and possibly the specific algo rithm being used.

## Transport Losses

While electrons moving in bulk material are subject to scattering and resistive losses, an electron confined to a portion of a helix at a suffciently low temperature is almost alvays in its ground state. The interactions between the electron and the lattice should be greatly diminished, particularly if the energy of the ground state is several times $k T$ below the energy of the first xcited state. Conventional resistive losses should be very greatly reduced.

It is important to distinguish between chage transport in helical logic and chage transport along a wire, even a very fine wire. The mobility of an electron confined to a one-dimensional wire c be much higher than in the bulk material(Sakaki 1980). However, even in this case the electron is confined in only two dimensions and can move freely along the third. In helical logic, by contrast, the electron is confined in all three dimensions. iewed from the frame of reference of the moing electron, it is simply sitting at the bottom of a potential well.

Lattice vibrations induced by the moving charge will cause transport losses. Treating the electron as an isolated charge subject to an oscillating force F, we have(Drexler 1992, page 164):

$$
P_{r a d} \approx F^{2} \omega^{2} \sqrt{\rho} \frac{1}{8 \pi M^{3 / 2}}
$$

$P_{\text {rad }}$ is the radiated power, $F$ is the force applied to the charge, $\omega$ is the frequency in radians per second, and M is a modulus of elasticity.

For an electric field E of $1^{8}$ volts/meter ( $10^{6}$ volts/centimeter, well below the breakdown strength of diamond) we have a force $F$ on a single electron of $1.6 \times 10^{-19} \times 10^{8}=1.6 \times 10^{-11} \mathrm{~N}$. The density $\rho$ of diamond is about $3,500 \mathrm{~kg} / \mathrm{m}^{3}$. The frequency $\omega$ in radians per second for a 100 picosecond time to make a single rotation is $2 \pi \times 10^{10}$. M is about $10^{12}$ Pascals. Substituting these values into equation (1) yields a radiated power of roughly $2.4 \times 10^{-18}$ watts, or $2.4 \times 10^{-28}$ joules per charge carrier per rotation of the electric field

This treats the electron as an isolated point chage, and also uses an approximation which should be accurate at frequencies well below the Debye frequency. The frequency selected is below the Debye frequency for diamond, while the error caused by the point charge assumption is conservative (in the sense that this assumption makes the energy dissipation higher than one would otherwise expect).

Lower power dissipation should be feasible. We could maintain approximate charge neutrality by placing a fi ed charge in the neighborhood of the electron. A donor atom contribting a positive charge will effectively cancel the negative charge of the electron. This is likely to produce a lower energy dissipation, as acoustic energy radiated from a dipole is lower than that radiated from a monopole (when the wavelength of the radiation is longer than the distance between the chages in the dipole). Alternatively, we could represent a logic " 1 " by the presence of an electroand a hole. The resulting dipole could then be transported along tho helices ("double helix logic") or both the electron and the hole could be confined in a single helix, one of them being half a turn ahead of th other. In the latter case, two types of dipole would be possible: one in which the electron precedes the hole, and another in which the hole precedes the electron. While it might appear paradoxical to have a helix which can simultanesouly confine both an electron and a hole, diamond helices wit fluorinated sur aces in vacuum should (as noted earlier) be able to do exactly that.

A frequency of $10^{10}$ hertz, along with the assumption that a single turn of the helix has a diameter of about 100 nanometers, implies that the electron is moing at a speed of about 3-4,000 meters per second (below the speed of sound in diamond). The dissipation mechanisms that might come into play for significantly higher speeds are not analyzed here

Accelerations caused by variations in the helical structure for the purpose of altering the direction of charge transport will result in accelerations of the chaged particle that might well result in radiative losses. Radiative losses are discussed further under switching losses, as accelerations of the charged particles during switching can likewise result in radiative losses.

## Dielectric Loss

The dielectric loss can be quite small. The highest experimental quality factor ( Q ) for a superconducting cavity resonator with a vacuum interior was $5 \times 10^{11}$ at a frequency of 10.5 GHz and a temperature of 1.3 K . Experimental values for Q for cavity resonators at low temperatures (a few Kelvins) with saphire interiors are above $10^{8}$ at a frequency of a few gigahertz, while Q's of $10^{15}$ are in principle feasible for defect-free saphire at 2 Kelvins and about 3 gigahertz(Braginsky 1985). For defect-free materials well below the Debye temperature, Q can increase as $1 / T^{5}$ or $1 / T^{4}$ as the temperature $T$ is decreased(Braginsky 1987, Gurevich 1979, Gurevich and Tagantsev 1991). It is reasonable to expect that the Q for defect-free diamond (a semiconductor which could be used for electronic devices) would be better than that for saphire. These results are for a solid block of homogeneous material, while an actual computer would have irregularities and inhomogenieties associated with the charge transport and switching devices, as well as the mobile charge carriers needed to propagate information. As a consequence, the Q for a computing device is likely to be different than the Q for a homogeneous material. Some analysis of this is done bekr, but this area requires futher investigation before definit ve statements about the dielectric loss for a real system can be made.

Dielectric losses for bulk silicon and diamond are described in (Braginsky 1985, Braginsky

1987, Gurevich 1979, Gurevich and Tagantsev 1991) by the equation:

$$
\tan \delta=\eta \frac{2 \pi \omega^{2}(k T)^{4}}{\varepsilon \rho v^{5} h\left(k T_{D}\right)^{2}}
$$

Where $\eta$ is a dimensionless anharmonicity parameter with typical values between 10 and 100 , $\omega$ is the frequency in radians per second, $\varepsilon$ is the dielectric permittivity of the crystal, $\rho$ the density, $h$ is Planck's constant, $v$ the speed of sound, $k$ is Boltzmann's constant, $T$ the temperature in Kelvins, and $T_{\mathrm{D}}$ the Debye temperature. Note that $\mathrm{Q} 1 /(\tan \delta)$.

In the case of diamond and approximating the value of $\eta$ as 100 (Braginsky 1987) we can approximate the loss factor. If we use $\omega=2 \pi \times 10^{10}, k=1.38 \times 10^{-23}, T=1 \mathrm{~K}, \varepsilon=5.7, \rho=3,510$ $\mathrm{kg} /$ meter $^{3}, h=6 \times 10^{-34}, T_{\mathrm{D}}=2340$, v $15,000 \mathrm{~m} / \mathrm{s}$; then we get $\tan \delta 10^{-20}$. (Experimental $\tan \delta$ 's for saphire of less than $10^{-9}$ at a frequency of about 10 gigahertz at a temperature of 1.5 Kelvins have been observed(Braginsky 1987). Saphire has a fundamentally higher tan $\delta$ because of its crystal symmetry). If we assume (rather generously) that each switch is a cube 100 nanometers on a side, and if we further assume that ten times this volume might be required for interconnections between switches (again rather generous), we have a total volume per switch of $10^{7}$ cubic nanometers. The energy stored by an electricic field of $1^{8}$ volts/meter in this volume results in an energy of about $2.5 \times 10^{-15}$ joules per gate (assuming a dielectric of 5.7, as before). Multiplied by our dielectric loss factor, we get an energy loss of under $10^{-34}$ joules per cycle per gate.

The form of the equation governing the dielectric loss varies greatly depending on the crystal symmetry. For example, centrosymmetric crystals of the $\mathrm{D}_{6 \mathrm{~h}}$ symmetry group have a dielectric loss that falls off as $\omega T^{9}$ (linear falloff in frequency, but ninth power in the temperature), while dielectric loss for crystals of the $\mathrm{C}_{\mathrm{i}}$ symmetry group falls off as $\omega^{5} T$ (Gurevich and Tagantsev 1991).

The presence of the helical paths creates a non-uniform structure, and hence induces additional losses. A loss mechanism suggested by Soreff(Soreff 1994) is caused by forces acting between induced dipoles. Even when charge carriers are completely absent the rotating electric field wil induce dipoles in the helical paths because the dielectric constant of the path and of the surrounding medium typically differ. A single half-turn of a helical path of the dimensions considered here can be approximated as a column about 100 nm long by 10 nm deep and 10 nm wide. If the electric field is $1^{8} \mathrm{v} / \mathrm{m}$ and we assume the disparity of the dielectric constants of the path and of the medium is approximately 5.7 (as would be the case for diamond helical paths), such a volume would have an induced dipole moment of roughly $5 \times 10^{-26} \mathrm{C}-\mathrm{m}$. Two such dipoles at a distance of roughly 100 nm (e.g., the opposing halves of a single helical turn) will experience a repulsive force of under $10^{-12} \mathrm{~N}$ (using a formula derived from the formula for the interaction energy given in (Israelachvili 1992)). Recall that the helical track is already being subjected to forces caused by the charge carrier, estimated above as $1.6 \times 10^{-11} \mathrm{~N}$, and that the energy dissipation is a function of the square of the force. Thus, the inter-track repulsive forces caused by induced dipoles are in this approximation smaller than the forces caused by a chage carrier by at least two orders of magnitude. Because the inter-track spacing is small compared with the acoustic wavelength, dissipation from this mechanism should be further substantially reduced. While the number of charge carriers is likely to be smaller than the number of helical turns, it is unlikly to be several orders of magnitude smaller.

The actual dielectric losses in a complex three dimensional structure consisting of numerous very small logic gates are certain to be diferent from the value estimated here for a perfect diamond crystal. However, it seems unlikely that such losses must necessarily be much larger and they can likely be made much smaller. The wide variation of dielectric loss among crystal types suggests that careful selection and design of materials can be used to male systems with very low dielectric losses. The uncertainty in the dielectric loss remains substantial, heever, and the actual loss could potentially be significantly higher than estimated here

## Switching Losses

Switching times need not be the same as the reciprocal of the clocking frequency. A single switching event could take place as the charges moved a fraction of a single helical turn, or could be spread out over many helical turns.

The reader who wants to think about a single specific geometry while reading the analysis in thi section can read the geometry of a specific switch gate in the first three paragraphs of the secti titled "Quantum Mechanical Analysis of the Operation of a Specific Switch Gate"

Switching losses occur because the two electrons are excited by their interaction and will dissipate energy when they fall back to their ground state. If we can keep the two electrons from entering an excited state, we can avoid energy dissipation.

A rather interesting observation is that switching losses caused by this mechanism can in principle be avoided almost completely even if the two electrons do enter excited states. An electron is in an "excited" state only with respect to some potential energy function. For any given wave function, however, there exists a potential energy function for which that wave function is the ground state. Thus, if we knew the wave function of each electron as it left the switch gate, and if we could engineer the path along which the electron mbes to have the appropriate potential enegy function, then the energy dissipated by the electron could in principle be eliminated.

Put more generally, if we know the state of a system then we need not (in principle) dissipate any energy at all.

Unfortunately, it would seem that the wave function of an electron leaving a switch gate depends on the presence or absence of the other electron. Even if both electrons entered the switch gate in their ground state, and even though the evolution of the wave function is deterministic, if we look only at one of the departing electrons we will find it in one of to states depending on the presence or absence of the other electron.

This can, in general, be solved by the use of the "interaction gate"(Fredkin and Toffoli 1982) illustrated in figure 7

In the interaction gate two electrons enter along two paths (A and B), and depart by four paths. Again, the interaction gate can be used to implement a Fredkin gate, and so it is logically complete. What makes the interaction gate interesting is the following property: if we know that an electron is present on a particular output path, then we know the inputs to the gate. For example, if an electron leaves the interaction gate along the A left path, then we know that there was an electron on path B (or else the electron would have left the gate on the A right path). Thus, we can engineer the precise geometry and potential of the A left path knowing exactly what state the electron is in

when it travels along that path.
Similar observations hold for all other ways in which an electron can leave the interaction gate, and so by appropriate engineering of the outgoing paths we can essentially eliminate eneigy dissipation from this source.

When a charge is switched down one of two alternate paths (as happens to the data electron in figure 6) it is subjected to an a guably unpredictable acceleration (we don't know which path it's going to take) which will in turn generate an arguably unpredictable pattern of radiation. If we assume that the accelerations involved are similar to those that would occur in an oscillating dipole, we can readily estimate the magnitude of this loss by using the formula for the power radiated by an oscillating point charge(Feynman 1963), page 32-3]:

$$
P_{r a d}=\frac{\omega^{4} q^{2} r^{2}}{12 \pi \varepsilon_{0} c^{3}}
$$

Dividing the radiated power by the frequency gives the energy dissipated per cycle, which is:

$$
\text { EnergyDissipated } / \text { cycle }=\frac{\omega^{3} q^{2} r^{2}}{6 \varepsilon_{0} c^{3}}
$$

For $\mathrm{f}=10$ gighertz and $\mathrm{r}=50$ nanometers (and nglecting the dielectric constant of the medium) this results in losses of about $10^{-35}$ joules per cycle.

Although this is a reasonable approximation to the enegy losses caused by the acceleration of a
single charge during the switching process, as noted earlier the switching frequency and the frequency of the externally applied electric field need not be xactly the same. Likewise, the distance which the switched and switching charges must traverse during a switching operation is different from the radius of the helix, and the acceleration profiles need not be sinusoidal. Furthe , modifi cations to the helical structure to transport chage carriers to various more or less random locations required by the computation will result in accelerations unrelated to switching.

Despite these admittedly rough approximations, the low dissipation computed suggests that this mechanism will not be the dominate source of energy dissipation under the conditions considered in this paper.

Because the energy dissipated per cycle is a function of the square of the charge, and because it might happen that many switches simultaneously switch charge in the same direction (thus effectively increasing the charge that is being accelerated) the energy dissipation from this mechanism might be increased significantl . This could be reduced by careful design of the switching operations to reduce the likelihood of such an event. Even stronger, if double helical logic is employed then a single switching operation could be so designed that it simultaneously accelerated both an electron and a hole in the same direction and by the same amount. This should effectively reduce energy dissipation from this mechanism by many orders of magnitude.

We assume that acoustic losses caused by the switching operation are similar to or smaller in magnitude than the acoustic losses caused by charge transport.

## Quantum Mechanical Analysis of the Operation of a Specific Switch Gate

## General

This analysis considers the behavior of a two-rail single-electron switch gate (figure 6). Note that the "two-rail" switch gate is similar to but distinctly different from the single-rail switch gate discussed earlier. In the two-rail variant, the single condition path is divided into two condition paths: a left condition path and a right condition path. There will always be one switching electron, entering either from the left or the right condition path. The switching electron is assumed to be in a narrow potential well that effectively confines it to a small region, assumed to be a point charge. The switched electron, by contrast, is assumed to be in a relatively wide harmonic potential, and it will be necessary to compute the wave function of the switched electron in this potential during the switching process. Although the switch gate is really a three dimensional structure, we will "unroll" the coordinate systems for this analysis. The z axis will measure "distance along the helix." The wave function of the switched electron is assumed to be confined to an $x-y$ plane at any given moment in time, although the z coordinate of the plane will move forwards as the switching process unfolds. The y coordinate for each path does not vary with time. The condition path is assumed to be a few nanometers "above" (located closer to the principal axis of the helix) the data path, i.e., the y coordinates of the data path and the condition path differ by a few nanometers. This implies that the x coordinates of the condition and data paths can vary independently with no risk that the two paths will collide and merge their contents.

This geometry can be visualized in the following way: think of the condition paths as being wrapped helically around one tube, and the data paths as being wrapped helically around a second tube of slightly larger diameter. Now, insert the smaller tube into the larger tube and align the
switching region of the data paths with the appropriate region of the condition paths. As the diameters of the two tubes are different, the electrons moving along a helical path on one tube can't move onto a helical path along the other tube. Only their electric fields will interact, allowing an electron on one tube to "push" the electron on the other tube down one of two alternative pathways.

Another way of thinking of the geometry of this switch gate starts by considering the diagrom of figure 6. Move the two condition paths above the plane of the paper (move the two condition paths towards you as you look at figure 6 -- this movement is orthogonal to the plane of the paper) by some short distance. This effectively moves the condition paths out of the plane of the data paths, and allows the condition and data paths to move up and down freely without any risk that they will collide and merge their contents. Note that "up" and "down" in this context are defined relative to figure 6 -- the switched data electron moving along the left path is moving "up". Finally, wrap figure 6 into a helical tube by raising the upper left and lower right corners towards each other.

The analysis that follows shows that a "plausible" potential exists which simultaneously provides a low energy dissipation and a low error rate at a reasonable switching speed. The underlying heuristic guiding its design was to minimize excitation of the switched electron during the switching process. The switched electron is assumed to have a significant probability of being excited, a probability which must be analyzed and minimized. Such excitation leads to both energy dissipation and to errors. By minimizing the excitation, both problems can be reduced.

The authors expect that significantly better potentials are feasible.
Standard SI units are used throughout.

## Slow switching

Slow switching processes in single-charge helical logic systems are straightforward: the underlying potential along the paths through the gate (determined by the structure of the device) evolves from one well to two, while the proximity of the switching charge raises the potential energy in the blocked path relative to that of the open path so that the ground state of the switched charge remains bound in the deeper well on the open path. In the limit of slow motion and low temperature, the probability of the charge remaining in the ground state can be made arbitrarily close to one, hence the probability of an error (which requires a higher energy state) can be made arbitrarily small. As will be seen, the energy difference between the ground state and the excited states that can evolve into states occupying the blocked well can be made to exceed $\Delta \mathrm{E}=10^{-21} \mathrm{~J}$, hence the probability that the blocked well will be occupied via thermal excitation [on the order of $\exp (-\Delta \mathrm{E} / \mathrm{kT})$ is less than $10^{-30}$ for temperatures of $\sim 1 \mathrm{~K}$. Accordingly, thermally induced errors can be made negligible. The chief source of errors in faster switching processes will be excitation resulting from nonadiabatic evolution of the system.

The switching time proposed is a few orders of magnitude slower than the period of a single oscillation of the switched electron when excited to the first excited state. This speed allows us to use the adiabatic approximation in computing the wave function of the switched electron, in estimating the probability of error, and in estimating the energy dissipation. Faster switching times should be feasible but would require a more detailed (and complex) analysis.

## Tailoring the potential function

Minimizing the error rate at a given switching speed requires accurate control of the underlying potential, achieved by some combination of bandgap engineering, modulation of well geometry, and manipulation of the local electrostatic environment (the distribution of charges, dipoles, and local dielectric constants). The following analysis assumes that the potential can be modulated by a tenth of an eV or more in essentially any smooth pattern. Analysis of a related problem (barrier heights of two surfaces sliding against each other) using a simple Monte Carlo technique makes this assumption plausible(Drexler 1992, page 278). For mathematical convenience, this analysis examines a potential with discontinuous first derivatives; smoother potentials (e.g., the present potential convolved with a suitable Gaussian) can have superior properties.

Variations in potential along the z axis are limited in frequency by the spacing of the atoms, and are further effectively limited by the fact the wave function will have some spread along the z axis. As a consequence, we have limited ourselves to a potential that varies relatively slowly with changes in the z coordinate. Variations in potential along the x axis involve tens of nanometers, and so could reasonably be engineered by appropriate placement of individual atoms. The potential along the $y$ axis is assumed to confine the electron to a fixed distance from the axis of the helix, e.g., the electron is confined to a helical ribbon.

## Non-thermal excitation and nearly-harmonic potentials

Each charge is assumed to be in its ground state as it enters the switch. An error is assumed to occur when a charge is excited to an energy level high enough to permit it to occupy a secondary potential well on the blocked path. (This is a conservative criterion: not all charges with sufficient energy will in fact exit along the blocked path.) For error rates to be low excitation probabilities must be small and the evolution of the system must be nearly adiabatic. An expression for the total probability of a transition from the $m$ th to the $n$th level under nearly-adiabatic conditions (Bohm 1951) is

$$
\left(P_{n}=\left|C_{n m}\right|^{2}\right) \cong \frac{4 \bar{h}}{\left(E_{n}-E_{m}\right)^{4}}\left|\int v^{*}{ }_{n} \frac{\partial H}{\partial t} v_{m} d x\right|^{2}
$$

where $P_{n}$ is the probability of ending in staten (assuming the initial state ism), $C_{n m}$ is the matrix element, $E$ is the energy of a state, $H$ is the system Hamiltonian, and $v_{n}$ and $v_{m}$ are wave functions. This gives an upper bound on the probability when the rate of change in the Hamiltonian $H / t)$ is a constant over some interval and zero before and after. Transition probabilities for systems in which $H / t$ increases and decreases smoothly over a timet $\gg(\overline{\mathrm{h}}) / \mathrm{E})$ are much lower; probabilities can also be larger or smaller after a series of abrupt changes, as phases add or cancel. For the present analysis, the maximum value of $P_{n}$ encountered in a series of sample times, $P_{n, \max }$, is used to estimate the probability of occupancy of that state at the end of that time interval. A more detailed analysis preserving phase information would be of interest, but should for the present system yield results of the same order as this estimate.

The following analysis describes the Hamiltonian and associated switched-charge wave functions along a one-dimensional coordinate. Wave functions are computed in the adiabatic approximation, neglecting the perturbing potential imposed by acceleration and charge mass (this imposed potential has a magnitude less than $5 \times 10^{23} \mathrm{~J}$, significantly smaller than the potentials imposed by either the switching charge or the material of the switch). Changes in this perturbing potential, however, provide a significant component of $\mathrm{H} / \mathrm{t}$ and hence substantially affect excitation probabilities.

We will call the potential created by the switch gate acting on the switched charge in the absence of the switching charge the "underlying potential." This potential is created by appropriate design of the switch gate. Because the switch gate is bilaterally symmetric, the underlying potential must necessarily be bilaterally symmetric as well.

Ideally, the switching charge would steer the switched charge down the chosen path without changing the shape of the potential well. From the frame of reference of the switched electron, almost nothing would have happened and excitation would be minimal. If the underlying potential were harmonic, and the potential imposed by the switching charge had a linear gradient, then the approach of the switching charge would have exactly this effect (a linear gradient applied to a harmonic well results in a new harmonic well of the same width but moved laterally: exactly what we desire).

In practice, the gradient created by a point charge is nonlinear. To some extent, this can be compensated by adjusting the underlying potential so that the resulting total potential (the underlying potential plus the potential created by the switching electron) is harmonic. This cannot be done completely, for the underlying potential is bilaterally symmetric and the wave function of the switched electron will have a significant component on both sides of the center of the switch gate (at least during the earlier phases of switching). However, the region of the underlying potential in the vicinity of the switched electron and on the same side of the centerline can be made exactly harmonic by appropriate modifications to the underlying potential. Second order terms can be cancelled by appropriate changes in the underlying potential, but higher-order terms cannot be cancelled during the early stages of switching, owing to the symmetry constraint on the underlying potential. (Effective cancellation of third-order terms becomes feasible when the switched charge has shifted by more than the characteristic radius of its ground-state wave function.) The residual sources of $H / t$ include third-order terms (during the early stages of switching), together with changes in the acceleration-induced potential and changes in the potential associated with the growth of a barrier as the incoming well in the underlying potential splits to form two outgoing wells.

## Structure of the potential

The potential surface analyzed here is not optimized, but is the product of several cycles of modification aimed at correcting obvious defects. The potential surface is defined in terms of two "paths," the path of the switching electron $\mathrm{x}_{\text {switching }}(\mathrm{z})$ and the path of the switched electron $\mathrm{x}_{\text {switched }}(\mathrm{z})$ (where z is a dimensionless quantity). While the path of the switching electron is exact, the "path" of the switched electron is only approximate as the wavefunction of the switched electron is diffuse in the x coordinate. The function $\mathrm{s}_{\text {witched }}(\mathrm{z})$ can therefore be viewed as an arbitrary function used to define the potential.

The potential combines several distinct components. The first is the electrostatic potential imposed by the switching charge:

$$
V_{\text {elect }}(x, z)=\frac{e}{4 \pi \varepsilon \varepsilon_{0}}\left[\Delta r^{2}+\left(x-x_{\text {switching }}(z)\right)^{2}\right]^{-\frac{1}{2}}
$$

We assume $\varepsilon$ is 5.7 (corresponding to the dielectric constant of diamond) andr is 4 nm (a gap in the $y$ direction sufficient to reduce cross-channel tunnelling to low values). The parameter $z$ is a dimensionless measure of distance along the path, entering into the dynamical analysis through a choice of $\mathrm{d} z / \mathrm{d} t$.

All other components are part of the underlying potential and are constrained to be even functions about the midpoint. These include a harmonic term:

$$
V_{\mathrm{harm}}(x)=\frac{1}{2} k_{s} x^{2}
$$

and a recursively-defined correction term

$$
\mathrm{V}_{\text {corr }}(\mathrm{x}, \mathrm{z})=\left\{\begin{array}{l}
\text { if }|\mathrm{x}|>2 \mathrm{x}_{\text {switched }}(\mathrm{z}), \mathrm{g}(\mathrm{z})|\mathrm{x}|-\mathrm{V}_{\text {elect }}(|\mathrm{x}|, \mathrm{z})+\mathrm{g}(\mathrm{z})\left|\mathrm{x}^{\prime}\right|-\mathrm{V}_{\text {elect }}\left(\left|\mathrm{x}^{\prime}\right|, \mathrm{z}\right) \\
\text { if }|\mathrm{x}| \leq 2 \mathrm{x}_{\text {switched }}(\mathrm{z}), \mathrm{g}(\mathrm{z})|\mathrm{x}|-\mathrm{V}_{\text {elect }}(|\mathrm{x}|, \mathrm{z})
\end{array}\right.
$$

where

$$
\mathrm{g}(\mathrm{z})=-k_{\mathrm{s}} x_{\text {switched }}(z) \text { and } x^{\prime}=2 x_{\text {switched }}(z)-|x|
$$

This term cancels the difference between the electrostatic potential and a linear gradient with a slope of $g \mathrm{~J} / \mathrm{m}$ in the region between $\mathrm{x}=0$ and $\mathrm{x}=2 x_{\text {switched }}(\mathrm{z})$, yielding a total potential that is exactly harmonic within these bounds. There does not appear to be a unique "right" choice for the value of the total potential outside these bounds. We have (somewhat arbitrarily) chosen the underlying potential so that $\left[V_{\text {total }}\left(x_{\text {switched }}(z)+\right.\right.$ offset, $\left.z\right)-V_{\text {total }}\left(x_{\text {switched }}(z), z\right)+\left[V_{\text {total }}\left(x_{\text {switched }}(z)\right.\right.$-offset, $z)-V_{\text {total }}\left(x_{\text {switched }}(z), z\right)=V_{\text {harm }}($ offset $)+V_{\text {harm }}(-$ offset $)$.

Finally, the walls of the potential well are steepened in regions where the ground state wave
function has a small amplitude by adding

$$
V_{\text {wall }}(\mathrm{x}, \mathrm{z})= \begin{cases}\text { if }|\mathrm{x}| \leq \mathrm{x}_{\text {switched }}(\mathrm{z})+9 \times 10^{-9} \mathrm{~m}, & 0 \\ \text { if }|\mathrm{x}|>\mathrm{x}_{\text {switched }}(\mathrm{z})+9 \times 10^{-9} \mathrm{~m}, & 10^{-3} \times\left[|\mathrm{x}|-\mathrm{x}_{\text {switched }}(\mathrm{z})-9 \times 10^{-9}\right]^{2}\end{cases}
$$

This term substantially raises the energies of the higher excited states without greatly affecting the ground state.

These various potentials have more or less randomly altered the potential at the bottom of the harmonic potential well, e.g., $V_{\text {total }}\left(x_{\text {switched }}(\mathrm{z}), \mathrm{z}\right)$ might vary as z varies. We desire, however, that the potential at the bottom of the well remain constant. To this end, we define $V_{\text {zero }}(\mathrm{z})$ as having that value required to make $V_{\text {total }}\left(x_{\text {switched }}(\mathrm{z}), \mathrm{z}\right)$ equal 0 . Note that $V_{\text {zero }}(\mathrm{z})$ is a function of z only and does not change as x changes.

The overall potential is:

$$
V_{\text {total }}(x, z)=V_{\text {harm }}(\mathrm{x})+V_{\text {elect }}(\mathrm{x}, \mathrm{z})+V_{\text {corr }}(\mathrm{x}, \mathrm{z})+V_{\text {wall }}(\mathrm{x}, \mathrm{z})+V_{\text {zero }}(\mathrm{z})
$$

The total potential has continuous first derivatives so long as the gradientg is numerically equal to $V_{\text {elect }}(x, z) / x$ evaluated at $x=0$. This condition can be maintained during the early evolution of the potential, but must be violated at later times. The difference between these gradients defines the magnitude of a wedge potential (creating a peak at $x=0$ ) that forms an implicit component of $V_{\text {total }}$.

## Time history of the potential

The evolution of the well potential determines $H / t$. Since the potential is determined by the positions of the switching and switched charges, the evolution of the well potential is specified by choices of $x_{\text {switching }}(z)$ and $x_{\text {switched }}(z)$. In the model potential, these functions are the natural cubic splines (Press et al. 1992) passing through the points tabulated in Table 1. The resulting paths and potentials are illustrated in Figures 9 and 10. The speed of switching is determined by $\mathrm{d} z / \mathrm{d} t$ (assumed to be constant). It is often convenient to use the reciprocal $\mathrm{d} t / \mathrm{d} z$, which we call the characteristic switching time or $t_{\text {char }}$. Figures 8,9 and 10 assume a $t_{\text {char }}$ of $5 \mathrm{ps}\left(\right.$ i.e., $\mathrm{d} z / \mathrm{d} t$ of $2 \times 10^{11}$ ).

Table 1. Defining points of natural cubic splines (Press et al. 1992) describing the trajectories of switched and switching charges in the model potential (rounded to three digit precision). The parameter $z$ is dimensionless.

Table 1:

| Switching |  | Switched |  |
| :--- | :--- | :--- | :--- |
| z | $\mathrm{x}(\mathrm{nm})$ | z | $\mathrm{x}(\mathrm{nm})$ |
| -2.0 | -100.0 | -2.0 | 0.105 |
| -1.0 | -50.0 | -1.0 | 0.418 |

Table 1:

| Switching |  | Switched |  |
| :--- | :--- | :--- | :--- |
| -0.6 | -32.0 | -0.65 | 0.872 |
| -0.25 | -15.5 | -0.6 | 1.01 |
| -0.1 | -11.0 | -0.25 | 4.0 |
| -0.05 | -9.9 | 0.0 | 10.0 |
| 0.2 | -15.3 | 0.4 | 24.5 |
| 0.3 | -19.6 | 2.0 | 130.0 |
| 0.6 | -33.8 |  |  |
| 1.0 | -57.2 |  |  |

In the initial (pre-wedge) phase of the switching interaction (through $z=\sim 0.05$ ), maintaining a zero wedge potential makes $x_{\text {switching }}$ and $x_{\text {switched }}$ functions of one another (a relationship approximated by the given splines). The acceleration profile is chosen to limit the the jerk resulting from the motion of the well minimum. (Note that the "wedge potential" is not an actual potential, but is merely a consequence of combining the potentials already defined. It is useful, however, to give it a name).

In the following (disengagement) phase, the growth of the wedge potential continues the motion of the switched charge away from the midplane, and a substantial and growing region around the well minimum is exactly harmonic. Changes in well shape outside this region cause residual excitation, but these decline as the exactly harmonic region expands into the tails of the ground-state wave function. (In particular, the discontinuity in the potential gradient associated with the peak of the wedge results in a fast rate of change of potential as seen in the well frame.) The disengagement phase ends as the magnitude of the ground-state wave function at $x=0$ becomes negligible (when $z$ 0.15).

In the final (seperation) phase, excitation is small, and (according to the energy-based error bound described above) errors are minimized by choosing a design that maximizes the quantum number $n$ of the lowest excited state centered in a secondary well. Placement of the switching charge so as to create two secondary wells of equal depths is nearly optimal during this phase; in the model potential, this condition determines $x_{\text {switching }}$ for $\mathrm{z}>0.2$. The lowest state that can become bound in the wrong well, $n=9$.

## Error rates

Error rates depend on $\mathrm{d} z / \mathrm{d} t$. Estimating error probabilities $P_{\text {err }}$ as the sum from $\mathrm{n}=9$ to $n=14$ of $P_{n \text {,max }}$, for values of $\mathrm{d} z / \mathrm{d} t$ corresponding to $t_{\text {char }}=5,10,20$, and 40 ps yields values of $\sim 9.3 \mathrm{x}$ $10^{-11}, 2.3 \times 10^{-11}, 5.8 \times 10^{-12}$, and $1.5 \times 10^{-12}$, respectively. Contributions from states with $n 15$ are small. The near proportionallity of $P_{\text {err }}$ to $(\mathrm{d} z / \mathrm{d} t)^{2}$ indicates that jerk contributes little to the excitation, which is instead dominated by consequences of deviations of ${ }_{\text {net }}$ from exact harmonicity. Even with $t_{\text {char }}=5 \mathrm{ps}, P_{\text {err }}$ remains low enough to enable the construction of digital logic systems
of high reliability, with a modest cost in time and energy dissipation resulting from error detection and correction.

## Energy dissipation due to switching

Energy dissipation occurs when switched charges undergo excitation and deexcitation (typically with phonon emission). This process is dominated by excitation $\mathrm{t} \boldsymbol{m}=1$, which is $>1 \hat{\theta}^{3}$ times more probable than excitation to any higher state. The associated energy dissipation $E_{\text {diss }} P_{1, \max } \times \overline{\mathrm{h}} \omega$ $P_{1, \max } \times 4.6 \times 10^{-22} \mathrm{~J}$. For $t_{\text {char }}=5,10,20$, and $40 \mathrm{ps}, E_{\text {diss }} 1.3 \times 10^{26}, 2.3 \times 10^{-28}, 1.7 \times 10^{-28}$, and $5.2 \times 10^{-29} \mathrm{~J}$ per switching event. Jerk plays a dominant role in energy dissipation-but not error rates-at the faster switching speeds, owing to the greater coupling to low-spatial-frequency features of $H / t$ by $n=1$, relative to $n 9$. Each of these values of $E_{\text {diss }}$ is far smaller than $k T$ at one $\operatorname{kelvin}\left(\sim 1.4 \times 10^{-23} \mathrm{~J}\right)$. An analysis retaining phase effects would permit the choice of an acceleration profile resulting in substantial cancellation of excitation to the $n=1$ state, reducing energy dissipation by $\sim 1000$ relative to the present estimates.

## Input and Output

Another issue is communication with the outside world. If the active computing element is embedded in a high intensity rotating electric field then the use of metallic wires poses ovious difficulties (much as placing a fork in a micr wave oven might be ill advised). It might still be possible to use wires provided that they are always at right angles to the electric field. It might $b$ difficult to achieve this, however, in which case some pickup from the rotating electric field ould still occur. The use of twisted pair would reduce this problem. Despite the obious drawbacks, the use of metallic wires might prove useful.

Another method would be to use fiber optics. This eliminates concerns about putting wires int an intense rotating electric field. Simply by $h$ ving an input fiber which started well outside th region of the rotating electric field and terminated within the act ve region it would be possible to selectively create electron-hole pairs in the semiconductor by injecting light into the other end of the fibe. Absorption of photons can be done in relatively small structures; for example, a one micron thickness of GaAs can absorb roughly a third of the incident light(Case and Panish 1978) page 46]. If the GaAs were part of a helical structure, the generated electrons and holesould then be separated by the electric field and ould move to opposite sides of the helix. This method of generating electron-hole pairs will produce packets of irregular size. By making too many electrons and holes and then selectively re-combining unwanted electrons and holes, we could reduce the packet size to the desired value. Re-combination will occur when the diameter of the helix becomes small enough to allow the electrons and holes to recombine. By controlling the diameter of the helix, the number of electrons and holes that remain in the packets can be controlled. An alternative method would be split the helix and allow the packet (through self repulsion) to break apart into smaller pieces. A sufficient number of splits would produce packets that had only a single electron or hole in them. The result would be several helices each one of which contained exactly zero or one charge carrier. This rather error-ridden input could then be converted into a more reliable result using appropriate logic circuitry.

Having once generated a pair of charge carriers, we could simply continue to let the pair be switched throughout further logic operations. Double helical logic would require the use of two
helical paths and two switching elements, increasing the volume and component complexity. By using single helical dipole logic (e.g., a single helix carrying both an electron and a hole to represent a " 1 ") the leading chage carrier would be switched through a switch gate and when the electric field rotated through an additional 180 degrees, the second carrier of the pair would be switched in exactly the same fashion.

For output, we need merely recombine electrons with holes next to an optical fibe. The optical fiber can then carry the resulting photons outside the rotating electric field where $c$ ventional detectors and electronics can be used. In single helix dipole logic, a simple method of combining electrons and holes would be to terminate a helical path carrying a pair The leading charge carrier, upon reaching the end of the helical path, would be unable to continue. The trailing carrier would then catch up. When the two met, the electron and hole would recombine and generate a photon.

Both input and output, depending on how they're implemented, might suffer from a relatively high error rate. This can be corrected by using various coding and multiple transmission schemes that provide sufficient redundan y to correct the errors.

Simple, robust I/O using optical methods should be feasible even in the presence of the strong rotating electric field required by helical logic

The optical methods of input and output described here are highly dissipative. Many entering photons will fail to generate an appropriate electron-hole pair; when a pair is generated in the electric field the resulting current f w will be dissipative; the recombination of electrons with holes to adjust the size of the charge packet is dissipative; and when electrons are combined with holes to generate optical output many of the resulting photons will be lost. While simple, this method of input and output is far from reversible and will impose energy limitations on the I/O bandwidth. It is often feasible in principle for I/O to be done in a reersible fashion. If two reversible processors wish to communicate with each other in a logically reersible manner, then there is no fundamental requirement that the process be dissipative. Further research is needed to provide a good low energy method of input and output.

Three main categories of energy dissipation were considered: transport losses, dielectric losses, and switching losses. Estimates of fundamental losses per cycle when the external field has a fre quency of 10 gigahertz were made. Transport losses are primarily acoustic, estimated at below $10^{-27}$ joules per cycle.

Dielectric losses vary widely depending on the exact crystal symmetry, with even the equation describing the loss being different for different symmetry groups. A rough estimate for the fundamental dielectric loss for diamond is below $10^{-35}$ joules per cycle per switch with an electric fiel strength of $10^{8}$ volts/meter. While pure diamond will almost certainly have a different (and lower) loss than the highly structured complex logic circuitry that would be needed in an actual system, this calculation still suggests that energy dissipation from this source can be made very small (and can likely be reduced to below $10^{-27}$ joules per cycle, the dissipation estimated from other loss mechanisms). Further research on the dielectric loss is required to better understand and minimize the losses that can be expected from this mechanism.

Switching losses below $10^{-27}$ joules per logic operation at switching speeds faster than $10^{-10} \mathrm{~s}$ should also be feasible. These losses involve both the excitation of electrons and their dissipative return to the ground state, as well as radiative losses resulting from the accelerations to which the
switched electron is subjected during a switching operation.
These estimates support the conclusion that thermodynamically reversible single electron logic operations should eventually be able to achieve very low energy dissipations, very likely below $10^{-27}$ joules per logic operation at a temperature of 1 K and a speed of 10 gigahertz. The largest energy loss mechanism identified as acoustic radiation, which could be reduced by the use of dipoles. Even though the estimates of dielectric loss and radiative loss were small there is substantial uncertainty in their values: further analysis seems appropriate.

## Faster Operation

The reader might have noticed that $10^{-27} \mathrm{~J}$ dissipated times $10^{-10}$ seconds switching time is $10^{-37}$ J -s, significantly bel w Planck's constant $h=6.626 \times 10^{-34} \mathrm{~J}$-s. This is not a violation of any fundamental principles, however(Feynman 1985). If, instead of the enegy dissipated we consider the magnitude of the change in the switching Hamiltonian $\Delta \mathrm{H}$ over the course of a switching operation then we can produce an enegy-time product which does have significance in the cont xt of the current proposal. The approximate value of $\Delta \mathrm{H}$ is $10^{-20} \mathrm{~J}$; multiplied by the switching time this gives $10^{-30} \mathrm{~J}$-s which is larger than Planck's constant by over three orders of magnitude. This gap suggests that faster switching should be feasible before any fundamental limits are encountered.

In the present proposal simply increasing the clock frequency would result in faster switching times, though at the cost of increased energy dissipation and error rate since no attempt was made to keep track of phase information. The switching time was simply made long compared with the time of a single oscillation of the first xcited state of the switched electron, thus allowing use of the adiabatic approximation. If the switching time were $-\Delta \mathrm{H} / h$ and if we computed the wave function of the switched electron as it left the switch, it should be possible to "catch" the switched electron in an appropriately designed potential. Switching speeds of $\sim 10^{-14} \mathrm{~s}$ with minimal energy dissipation and error rates should be feasible using this approach. With lateral movement of the switched electron of $\sim 10^{-8} \mathrm{~m}$ we have electron speeds of $\sim 10^{6} \mathrm{~m} / \mathrm{s}(\sim .003 \mathrm{c})$, accelerations of $\sim 1 \boldsymbol{\vartheta}^{0}$ $\mathrm{m} / \mathrm{s}^{2}$, forces of $\sim 10^{-11} \mathrm{~N}$, and an electron-electron separation (in vacuum) of $\sim 5 \times 10^{-9} \mathrm{~m}$. Relativistic effects and materials limitations should not pose fundamental limitations for operations at these speeds.

A switching speed faster than $\sim 10^{-14} \mathrm{~s}$ in the context of the current proposal would require creating a larger switching potential by, for example, using more than one switching electron (e.g., a charge packet). Use of a suitable charge packet would also permit reliable room temperature operation. More detailed analysis of rapid switching would be of interest.

## Summary

The picture of computing that emerges from this analysis is relatively simple: a solid block of material that is intricately designed at the molecular level is placed into a cavity resonator which has a frequency of several gigahertz. The resonator and the block of material are kept at low temperature, perhaps 1 K . Fiber optic connections allow the block to communicate with the outside world. Photons generated outside the cavity resonator by conventional electronics are carried into the block via fiber optics to create electron hole pairs, which then enter into computations withi the block. By combining electrons with holes, photons can be generated within the block which are then carried out of the caity resonator by fiber optics and detected by coventional electronics.

The cavity resonator has a high Q , and the computations within the block of material produce relatively little additional energy loss. A significant source of ene gy loss in this particular proposal is in the I/O, which is quite dissipative. If the number of I/O operations is relatively small compared with the number of total logic operations performed or if some method of I/O can be found which dissipates much less energy (which seems likely) then the total energy dissipation per logic operation can be made remarkably small.

## Conclusions

Projections of current trends in energy dissipation per gate operation(Landauer 1988) suggest that the $k T$ "barrier" will become significant within a few decades. This barrier can be overcome by using reversible logic. Further, the trend towards decreasing device size and increasing device precision will likely result in atomically precise logic elements which employ single electrons, single holes, or both to carry the 0 's and 1 's of a computation. Helical logic is the first proposed member of the class of single electron thermodynamically reversible atomically precise logic devices. Members of this class might mark the ultimate evolution of electronic devices. Helical logic also avoids many of the problems of conventional clock distribution. The energetic costs of charging and discharging clock lines might otherwise become a significant source of energy dissipation in future computing devices. A preliminary analysis suggests that the energy dissipation of helical logic can be reduced below $10^{-27}$ joules per logic operation at a switching speed of 10 gigahertz and an operating temperature of 1 K . Further reductions in energy dissipation might be feasible if double helical logic is used. The estimates of dielectric loss and radiative loss were both well below $10^{-27} \mathrm{~J}$, but had significant uncertainties that require further examination. Further research to develop the highly precise manufacturing technologies needed to economically fabricate this (and other) proposed computing technologies is needed(Merkle 1994). Further investigation of single electron, thermodynamically reversible, atomically precise logic devices seems warranted.

## Acknowledgements

The authors would like to thank J. Storrs Hall, Rolf Landauer, Alan Lewis, Norman Margolus, Jim Mikkelsen, John Northrup, Ed Richley, Jeff Soreff, Robert Thornton, Tommaso Toffoli, and Chris van de Walle.

## References

Bean, J. C. (1992) Proceedings of the IEEE, Vol. 80 No. 4, April. Silicon-Based Semiconductor Heterostructures: Column IV Bandgap Engineering

Bennett, C. H. (1973) IBM Journal of Research and Development, 17, 525-532, November. Logical Reversibility of Computation

Bennett, C. H. (1982) International Journal of Theoretical Physics, Vol. 21, No. 12 905-940. The Thermodynamics of Computation - A Review

Bennett, C. H. and Landauer, R. (1985) Scientific American, July, 4856. The Fundamental Physical Limits of Computation

Bennett, C. H. (1988) IBM J. Research and Development, Vol. 32, No. 1, January, 16 -23. Notes
on the History of Reversible Computation
Bennett, C.H. (1989) SIAM J. Computing, Vol. 18, No. 4, 766 -776, August. Time/Space Trade-offs for Reversible Computation

Bobeck, A. H. and Scovil, H.E.D. (1971) Scientific American, June, Vol. 224, No. 6, 78-91. Magnetic Bubbles

Bohm, D. (1951) Quantum Theory (Prentice Hall).
Braginsky, V. B., Mitrofanov, V. P. and Panov, V. I. (1985)Systems with Small Dissipation (University of Chicago Press).

Braginsky, V. B., Ilchenko, V. S., and Bagdassarov, Kh. S. (1987) Physics Letters A, Volume 160, No. 6, March 2, 300-305. Experimental observation of fundamental microwave absorption in high-quality dielectric crystals

Carter, F.L, Siatkowski, R.E. and Wohltjen, H. eds., (1988) Proceedings of the 3rd International Symposium on Molecular Electronic Devices (North-Holland).

Casey H. C. and Panish, M. B. (1978) Heterostructure Lasers (Academic Press).
Drexler, K. E. (1988) in Proceedings of the 3rd International Symposium on Molecular Electronic Devices, F.L. Carter, R.E. Siatkowski, H. Wohltjen, eds. (NorthHolland). Rod Logic and Thermal Noise in the Mechanical Nanocomputer

Drexler, K.E. (1992) Nanosystems: Molecular Machinery, Manufacturing, and Computation (Wiley Interscience).

Feynman, R.P. (1960) Caltech's Engineering and Science, February. Also see http://nano.xerox.com/nanotech/feynman.html. There's Plenty of Room at the Bottom

Feynman, R. P., Leighton, R. and Sands, M. (1963) (Addison Wesley). The Feynman Lectures on Physics, Vol. I

Feynman, R. P. (1985) Optics News, February, 11-20. Quantum Mechanical Computers
Fredkin, E. and Toffoli, T. (1978) November 1978 DARPA proposal. Design Principles for Achieving High-Performance Submicron Digital Technologies

Fredkin E. and Toffoli, T. (1982) International Journal of Theoretical Physics, Vol. 21, Nos. 3/4, 219-253. Conservative Logic

Grabert H. and Devoret M. H. (eds) (1992) Single Charge Tunneling (Plenum Press)
Gurevich, V. L. (1979) Sov. Phys. Solid State 21(11), November, 1993-1998.Dielectric Losses in Crystals

Gurevich, V. L. and Tagantsev, A. K. (1991) Advances in Physics, Vol. 40, No. 6, 719-767Intrinsic dielectric loss in crystals

Hall, J.S. (1992) Laboratory for Computer Science Research, Rutgers University, Proceedings of the Workshop on Physics and Computation, October 2-4, 237-247 (IEEE Press). Electroid Switching Model for Reversible Computer Architectures

Halliday, D. and Resnick, R. (1988) The Fundamentals of Physics, Extended Third Edition (Wiley).

Israelachvili, J. (1992) Intermolecular and surface forces, second ed. (Academic Press)
Kinoshita, K., Sasao, T. and Matsuda, J. (1976) IEEE Transactions on Computers, Vol. C-25, No. 3, March, 247-253. On Magnetic Bubble Logic Circuits

Koller, J. G. and Athas, W. C. (1992) Proceedings of the Workshop on Physics and Computation, October 2-4, 267-270 (IEEE Press). Adiabatic Switching, Low Energy Computing, and the Physics of Storing and Erasing Information

Landauer, R. (1961) IBM Journal of Research and Development, Vol. 6, July 1961, 183-191. Irreversibility and Heat Generation in the Computing Process

Landauer, R. (1981) in Sixth International Conference on Noise in Physical Systems, Mejier, P.H.E., Mountain, R. D., Soulen Jr., F. J. eds [Nat. Bur. Stand. (U.S.), Publ. 614] 12Fundamental Physical Limitations of the Computational Process

Landauer, R. (1988) Nature, Vol. 335, October 27, 779. Dissipation and noise immunity in computation and communication

Likharev, K. K. (1982) International Journal of Theoretical Physics, Vol. 21, Nos 3/4, 311 to 326. Classical and Quantum Limitations on Energy Consumption in Computation

Likharev, K. K. and Claeson, T (1992) Scientific American Vol 266 No. 6, June, 80 -85. Single Electronics

Likharev, K. K., Rylov, S. V. and Semenov, M. K. (1985) IEEE Transactions on Magnetics, Vol. MAG-21, No. 2, March, 947-950. Reversible Conveyer Computation in Array of Parametric Quantrons

Merkle, R. C. (1992) Proceedings of the Workshop on Physics and Computation, October 2-4, 227-228 (IEEE Press). Towards Practical Reversible Logic

Merkle, R. C. (1993a) Nanotechnology 4, 86-90. A Proof about Molecular Bearings
Merkle, R.C. (1993b) Nanotechnology 4 114-131. Two Types Of Mechanical Reversible Logic
Merkle, R. C. (1993c) Nanotechnology 4, 21-40. Reversible Electronic Logic Using Switches
Merkle, R. C. (1994) in:The Ultimate Limits of Fabrication and Measurement, Welland, M. E. and Gimzewski, J. K. eds. (Kluwer, Dordrecht). Self Replicating Systems and Low Cost Manufacturing

Press W. H., Teukolsky S. A., Vetterling W. T., and Flannery B.P. (1992) (Cambridge University Press). Numerical Recipes in FORTRAN: the art of scientific computing, second ed.

Ressler, A.L. (1981) Master's Thesis, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, January.The Design of a Conservative Logic Computer and a Graphical Editor Simulator

Sakaki, H. (1980) Japanese Journal of Applied Physics, Vol. 19 No. 12, December, L735-L738.

Scattering Suppression and High-Mobility Effect of Size-Quantized Electrons in Ultrafine Semiconductor Wire Structures

Seitz, C. L., Frey, A. H., Mattisson, S., Rabin, S. D., Speck, D. A., van de Sneepscheut, Jan L. A. (1985) Chapel Hill Conference on VLSI, Computer Science Press, 1 -17. Hot-Clock nMOS

Soreff, J. (1994) private communication.
Sze, S. M.(1990) High-Speed Semiconductor Devices (Wiley Interscience).
Van de Walle, C. G. (1989) Physical Review B, volume 39, Number 3, January 15, II, 1871-1883. Band lineups and deformation potentials in the model-solid theory

Washburn, S. (1992) Nature Vol 357, May 21, 199-200. Single atoms as transistors
Younis, S. G. and Knight, T. (1993) AI Laboratory, MIT, preprint. Practical Implementation of Charge Recovering Asymptotically Zero Power CMOS

