

# NMR Quantum Computation with a hyperpolarized nuclear spin bulk

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## Abstract

We consider two new quantum gate mechanisms based on nuclear spins in hyperpolarized solid  $^{129}\text{Xe}$  and HCl mixtures and inorganic semiconductors. We propose two schemes for implementing a controlled NOT ( CNOT ) gate based on nuclear magnetic resonance ( NMR ) spectroscopy and magnetic resonance imaging ( MRI ) from hyperpolarized solid  $^{129}\text{Xe}$  and HCl mixtures and optically pumped NMR in semiconductors. Such gates might be built up with particular spins addressable based on MRI techniques and optical pumping and optical detection techniques. The schemes could be useful for implementing actual quantum computers in terms of a cellular automata architecture.

## 1 Introduction

The study of quantum computation has attracted considerable attention since Shor discovered a quantum mechanical algorithm for factorization in polynomial instead of exponential time [1] in 1994. In 1996, Grover [2] also showed that quantum mechanics can speed up a range of search applications over an unsorted list of  $N$  elements. Hence it appears that a quantum computer can obtain the result with certainty in  $O(\sqrt{N})$  instead of  $O(N)$  attempts.

In 1982, Benioff [3] showed that a computer could in principle work in a purely quantum-mechanical fashion. In 1982 and 1986, Feynman showed

that a quantum computer might simulate quantum systems [4] [5]. In 1985 and 1989, Deutsch [6] [7] first explicitly studied the question that quantum-mechanical processes allow new types of information processing. Quantum computers have two advantages. One is the quantum states can represent a 1 or a 0, or a superposition of a 1 and a 0, which leads to quantum parallelism computations. The other is quantum computers perform deterministic unitary transformations on the quantum states.

It is difficult to build up quantum computers for two principal reasons. One is decoherence of the quantum states. The other is a quantum computer might be prone to errors, which are troublesomely corrected. The current developments, however, have showed that the two obstacles might be surmounted. Shor [8] [9] and Steane [10] discovered that the use of quantum error-correcting codes enables quantum computer to operate in spite of some degree of decoherence and errors, which may make quantum computers experimentally realizable. Knill et al. [11] also showed that arbitrary accurate quantum computation is possible provided that the error per operation is below a threshold value. In addition, it is possible to decrease the influence of decoherences by using mixed-state ensembles rather than isolated systems in a pure state [12] [13] [14].

Among many candidate physical systems envisioned to perform quantum computations (such as quantum dots [15] [16], isolated nuclear spin [17], trapped ions [18], optical photons [19], cavity quantum-electrodynamics [20] [21] and nuclear magnetic resonance (NMR) of molecules in a room temperature solution [12] [13] etc.), NMR quantum computers [12] [13] are particularly attractive because nuclear spins are extremely well isolated from their environment and readily manipulated with modern NMR methods. Recently, Chuang and Jones et al. [22] [23] have experimentally realized for the first time a significant quantum computing algorithm using NMR techniques to perform Grover's quantum search algorithm [2]. In addition, NMR quantum computers with two qubits or three qubits have been used to implement Deutsch's quantum algorithm [24] [25] [26]. Cory et al. have experimentally realized for the first time quantum error correction for phase errors on an NMR quantum computer [27]. However, there are two primary challenges in using nuclear spins in quantum computers. One is low sensitivity of NMR signals. The other is that scaling-up to much larger systems with this approach may be difficult [28]. Recently, Kane [29] has presented a scheme for implementing a quantum computer, using semiconductor physics to manipulate nuclear spins. This may be an answer to scaling up to produce

useful quantum computers [30]. However, the current technology is difficult to implement Kane's scheme [29] [30].

Chuang *et al.* first experimentally demonstrated the complete model of a simple quantum computer by NMR spectroscopy on the small organic molecule chloroform [22]. Their experimental results showed that the execution of certain tasks on a quantum computer indeed requires fewer steps than on a classical computer. However, building a practical quantum computer by the use of NMR techniques poses a formidable challenge. Steps of circumventing these problems based on the bulk spin resonance approach to build quantum computers can include increasing the sample size, using coherence transfer to and from electrons, and optical pumping to cool the spin system [31].

DiVincenzo *et al.* have suggested that a "solid state" approach to quantum computation with a  $10^6$  qubit might be possible [16]. Solid-state devices open up the possibility of actual quantum computers having realistic applications [30]. In the paper, we shall discuss the implementation of a controlled NOT gate between two spins with a spin-hyperpolarized bulk. It should be noted that an important progress in optical pumping in solid state nuclear magnetic resonance (OPNMR) has been made [32]. Recently, interest has been growing in exploitation of optical pumping of nuclear spin polarizations as a means of enhancing and localizing NMR signals in solid state nuclear magnetic resonance [32]. The principal work has been concentrated in the following two areas. The polarization of  $^{129}\text{Xe}$  can be enormously enhanced through spin-exchange with optically pumped alkali-metal vapor [33]. The NMR signals from  $^{129}\text{Xe}$  nuclei have enhanced to  $\sim 10^5$  times the thermal equilibrium value [33]. The spin-lattice relaxation of the  $^{129}\text{Xe}$  nuclei in the polarized solid  $^{129}\text{Xe}$  is exceptionally slow (such as relaxation times longer than 500h [34]). In addition, the experimental results [34] [35] [36] [37] [38] have shown that laser-polarized  $^{129}\text{Xe}$  nuclei can be used to polarize other nuclei that are present in the lattice or on a surface through cross relaxation or cross polarization. Optical pumping NMR (OPNMR) techniques of inorganic semiconductors (such as GaAs, and InP *et al.*) [32] at low temperatures can enhance NMR signals in solids, which can circumvent the two problems in solid state NMR, that is, its relative low sensitivity and its lack of spatial selectivity. In OPNMR, spatial localization of the NMR signals can be achieved through spatial localization of the optical absorption and through cross polarization or relaxation mechanisms [32] [39] [40]. In this paper, we shall propose two schemes for implementing a controlled NOT (CNOT) gate

in quantum computers based on NMR spectroscopy and magnetic resonance imaging from hyperpolarized solid  $^{129}\text{Xe}$  and HCl mixtures and OPNMR in the solid state nuclear magnetic resonance of inorganic semiconductors ( quantum well and quantum dot ).

The paper is organized as follows. In Sec.II, we introduce the model for the controlled NOT gates in terms of hyperpolarized solid  $^{129}\text{Xe}$  and HCl mixtures. In Sec.III we present a scheme for implementing a CNOT gate based on OPNMR in inorganic semiconductors. In Sec.IV, we present implications for experiments on our schemes.

## 2 Quantum computation with hyperpolarized $^{129}\text{Xe}$ and HCl solid mixtures

To realize quantum computation, it is necessary to have the nonlinear interactions in a system. These nonlinear interactions can simultaneously be influenced externally in order to control states of the system. Meanwhile, it is required that the system can be extremely well isolated from its environment so that the quantum coherence in computing is not rapidly lost. In a solid, there are dipolar couplings between two spin systems, which result in broader NMR lines and cross relaxation among spin systems. The interactions in solids can be controlled with complex radio-frequency (rf) pulse sequences (such as decoupling pulse sequences). In general, the interactions in solids are so strong that the eigenstates are not the simple spin product states and logical manipulation are more complex [28]. However, for special solids (such as  $^{129}\text{Xe}$  and  $^1\text{HCl}$ , and  $^{129}\text{Xe}$  and  $^{13}\text{CO}_2$  mixtures), since the homonuclear spin system is diluted by other spin system, the spin dipolar interactions between two homonuclei are weak and the solid mixtures may be homogeneous so that the solids could have a resolved dipolar structure. A full quantum mechanical treatment of the spin system is in order [41].

Spin-exchange optical pumping can produce hyperpolarized  $^{129}\text{Xe}$  (with an enhanced factor of about  $10^5$ ) [33]. The hyperpolarized  $^{129}\text{Xe}$  gas can be frozen into a hyperpolarized  $^{129}\text{Xe}$  solid with little or no loss of  $^{129}\text{Xe}$  nuclear spin polarization [34]. It should be noted that nuclear spin polarization of  $^{129}\text{Xe}$ , which is produced with spin-exchange optical pumping, does not depend on the strength of magnetic fields. Therefore, the NMR experiments can be performed in low fields produced by the general electromagnets or

the magneto irons. NMR signals with sufficient signal-to-noise ratio from a hyperpolarized  $^{129}\text{Xe}$  solid are available on a single acquisition. At low temperatures, the spin-lattice relaxation of the  $^{129}\text{Xe}$  nuclei in the hyperpolarized solids is extremely slow. For example, the  $^{129}\text{Xe}$  spin polarization lifetime  $T_1$  is hundreds of hours at 1 KG below 20K [34]. Linewidth of NMR signals from a hyperpolarized  $^{129}\text{Xe}$  solid is tens of Hz [42]. This indicates that the  $^{129}\text{Xe}$  nuclei in a hyperpolarized solid can be relatively well isolated from their environment. Through dipolar-dipolar interactions, enhanced nuclear spin polarization of  $^{129}\text{Xe}$  can be transferred to other nuclei ( $^1\text{H}$  and  $^{13}\text{C}$  etc.) on a surface [37] [36], in a solid lattice [35] [34] and a solution [38]. The experimental results have indirectly shown that the sign of the  $^{129}\text{Xe}$  polarization can be controlled by the helicity of the pumping laser or the orientation of the magnetic field in the optical pumping stage [35] [38]. It is interesting to note that the signs of polarization of other nuclei ( $^1\text{H}$  and  $^{13}\text{C}$ ) depend on those of polarization of  $^{129}\text{Xe}$  nuclei in the cross polarization experiments [35] [38]. The signs of polarization of other nuclei ( $^1\text{H}$  and  $^{13}\text{C}$ ) are the same as  $^{129}\text{Xe}$  nuclei [35] [38].

In quantum computation, Barenco *et al.* [43] have shown that single-spin rotations and the two-qubit "controlled"-NOT gates can be built up into quantum logic gates having any logical functions. In the following, we shall show how to build up a "controlled" NOT gate based on NMR signals from a hyperpolarized  $^{129}\text{Xe}$  solid.

Before our discussions, we first show how to prepare a hyperpolarized  $^{129}\text{Xe}$  and HCl solid mixture. First, spin-exchange optical pumping produces hyperpolarized  $^{129}\text{Xe}$  gas at a 25G magnetic field. Secondly, the polarized xenon is mixed with 760 Torr of HCl at room temperature and the mixture is rapidly frozen into the sample tube in liquid  $N_2$ .

In solids, the dominant mechanism of spin-spin relaxation is the dipole-dipole interaction. The experimental results [35] [38] [36] have shown that the transfer of a large nuclear polarization from  $^{129}\text{Xe}$  to  $^1\text{H}$  (or  $^{13}\text{C}$ ) can be controlled by cross polarization techniques in the solids. Hyperpolarized  $^{129}\text{Xe}$  ice can be used to polarize  $^{131}\text{Xe}$  [34] and  $^{13}\text{C}$  ( $\text{CO}_2$ ) [35] trapped in the xenon lattice through thermal mixture in low fields. Pines *et al.* [37] have shown that high-field cross polarization methods can make magnetization transfer between two heteronuclear spin systems selective and sensitive.

In a quantum computer, logic functions are essentially classical, only quantum bits are of quantum characteristic (quantum superpositions) [2]. In the  $^{129}\text{Xe}$  and HCl solid mixture, one can use complex pulse sequences and

dipole-dipole interactions between  $^{129}\text{Xe}$  and  $^1\text{H}$  to manipulate and control two qubits ( $^{129}\text{Xe}$  and  $^1\text{H}$ ). In the following, we shall discuss the scheme for implementing a controlled NOT (CNOT) gate in quantum computers based on NMR spectroscopy and magnetic resonance imaging from the hyperpolarized solid  $^{129}\text{Xe}$  and HCl mixtures.

Since  $^{129}\text{Xe}$  and  $^1\text{H}$  in the solid are a weakly-coupled two-spin IS system with a resolved structure, in the doubly rotating frame, rotating at the frequencies of the two applied r.f. fields, the Hamiltonian of this system can be written as [41]

$$\mathbf{H} = \Omega_I I_z + \Omega_S S_z + 2\pi J_{IS} I_z S_z + \omega_{1I} I_x + \omega_{1S} S_x$$

where  $\Omega_I$  and  $\Omega_S$  are the resonance offsets, and  $\omega_{1I}$  and  $\omega_{1S}$  are the two r.f. field strengths, respectively.  $\omega_{1I}$  and  $\omega_{1S}$  can be used to perform arbitrary single-spin rotations to each of the two spins (I and S) with selective pulses [41].

In the above Hamiltonian, the Hamiltonian  $\mathbf{H}_{IS} = 2\pi J_{IS} I_z S_z$  leads to the following evolution operator

$$\widehat{R}_{zIS}(J_{IS}\tau\pi) = e^{i2\pi J_{IS}\tau I_z S_z}$$

$$= \cos(J_{IS}\tau\pi/2) + i \sin(J_{IS}\tau\pi/2) \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{vmatrix}.$$

$$\text{when } \tau = \frac{1}{2J_{IS}}, \widehat{R}_{zIS}(J_{IS}\tau\pi) = \frac{\sqrt{2}}{2} \begin{vmatrix} 1+i & 0 & 0 & 0 \\ 0 & 1-i & 0 & 0 \\ 0 & 0 & 1-i & 0 \\ 0 & 0 & 0 & 1+i \end{vmatrix}.$$

It is easy to perform single-spin rotations with arbitrary phase  $\phi$  with the modern pulse NMR techniques [41]. For example, one can perform single-spin rotations via composite z-pulses [44] and free precession [25].

In the ideal case, the operator to perform CNOT gates can be written as

$$\widehat{C}_{CNOT} = \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{vmatrix}.$$

A "controlled" NOT gate can be realized by the following pulse sequences [13] [31]

$$\widehat{C}_{1AB} = \widehat{R}_{yA}(-\pi/2)\widehat{R}_{zB}(-\pi/2)\widehat{R}_{zA}(-\pi/2)\widehat{R}_{zAB}(\pi/2)\widehat{R}_{yA}(\pi/2)$$

$$= \sqrt{-i} \begin{vmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{vmatrix} \quad (1),$$

$$\begin{aligned} \text{or} \\ \widehat{C}_{2AB} &= \widehat{R}_{yB}(\pi/2) \widehat{R}_{zAB}(\pi/2) \widehat{R}_{xB}(\pi/2) \\ &= \begin{vmatrix} (-1)^{1/4} & 0 & 0 & 0 \\ 0 & -(-1)^{3/4} & 0 & 0 \\ 0 & 0 & 0 & (-1)^{1/4} \\ 0 & 0 & (-1)^{3/4} & 0 \end{vmatrix} \quad (2), \end{aligned}$$

where A and B represent "target" qubit ( $^1H$  (HCl)) and "control" qubit ( $^{129}Xe$ ), respectively. In eq. (1), one can not only apply composite z-pulses [44] actively to perform  $\widehat{R}_{zA}(-\pi/2)$  and  $\widehat{R}_{zB}(-\pi/2)$  but also let a two-spin AB system freely evolve in periods of precession under Zeeman Hamiltonians. When using pulse-sequences in Eqs. (1) and (2), one can obtain a similar effect on quantum computation [31]. This involves an important problem, that is, optimized rf pulse sequences. It is important to eliminate unnecessary pulses.

The CNOT operations can also be performed on the basis of the cross-polarization experiments in solid state NMR. Under some experimental conditions, one uses pumping laser with helicities  $\sigma^-$  and  $\sigma^+$  to produce positive or negative polarizations of  $^{129}Xe$  through spin-exchange laser pumping techniques before one performs the CNOT operations. If polarization of  $^{129}Xe$  nuclei is negative, no operation is needed. If polarizations of  $^{129}Xe$  nuclei and  $^1H$  nuclei are positive, one can use the cross-polarization pulse sequences shown in Fig.1a to perform the controlled rotation operations. If polarizations of  $^{129}Xe$  nuclei and  $^1H$  nuclei are respectively positive and negative, one can use the pulse sequences in Fig.1b to perform the CNOT gate operations.

In order to yield a large sensitivity enhanced for  $^1H$ , before performing CNOT gates, we perform cross polarization experiments of the  $^1H$  and  $^{129}Xe$  system. In addition, in order to enhance sensitivity of NMR signals, one can selectively consider a hyperpolarized  $^{129}Xe$  and a  $^1H$  as the "target" qubit and the "control" qubit respectively. If we use three types of gases ( $^{129}Xe$ ,  $^1HCl$  and  $^{13}CO_2$ ) to prepare the NMR sample, we can perform quantum logic gates with three qubit ( $^{129}Xe$ ,  $^1H$  and  $^{13}C$ ). If we respectively use different pressures of  $^{129}Xe$ ,  $^1HCl$  and  $^{13}CO_2$ , we can increase or decrease the homonuclear dipole-dipole interaction. That is because when the relative pressure of the other gases is increased or decreased, the distance r between

two homonuclei is increased or decreased.

As we know, the principal limitation of solid state NMR is its relatively low sensitivity. In addition, another limitation of solid state NMR is its lack of spatial selectivity and extremely broad NMR lines. This is because the NMR signals from an inhomogeneous sample are bulk-averaged [32] and the dipole-dipole interactions between two spins are strong. Therefore, it is difficult to assign particular logic gates to regions within the bulk sample. Constructing the actual quantum circuit based on NMR could be an important issue. Now, the actual quantum circuit based on liquid state NMR is constructed only *in time* by using different pulse sequences. Can we build up actual quantum circuits both *in time* and *in space*? It is interesting to note that NMR signals from  $^{129}\text{Xe}$  ice have relatively high sensitivity and that NMR lines are relatively narrow [42]. It is possible to construct the actual quantum circuit based on hyperpolarized  $^{129}\text{Xe}$  ice *in space* using magnetic resonance imaging (MRI) and NMR spectroscopy techniques. If one uses gradient fields [12], one can make the quantum logic gates localized in space in a bulk sample. Therefore logic gates having any logical functions can be performed not only *in space* but also *in time*. Entanglement between spins of two different cells may be realized by homonuclear spin diffusion.

### 3 Quantum computation based on optically pumped NMR of semiconductors

Recently, great progress in optically pumped NMR (OPNMR) in semiconductors, single quantum dot, as well as quantum wells has been made [32] [39] [40]. An optical pumping technique can be used to enhance and localize nuclear magnetic resonance signals. This method has greatly improved spatial resolution and sensitivity of NMR signals.

Spatial localization of the NMR signals from solids can be achieved through spatial localization of the optical absorption and through subsequent manipulations and transfers of the optically pumped nuclear spin polarization [32].

Enhanced NMR signals can be detected either indirectly by optical techniques [32] or directly by conventional rf pick up coils [32]. Optical detection can extremely sensitively measure NMR signals from a single quantum dot ( $\leq 10^4$  nuclei) [39]. Here we propose a scheme for the implementation of quantum logic gates by using OPNMR in solids, where the electron spin  $\vec{S}$



and the nuclear spin  $\vec{T}$  are respectively considered as the “control” qubit and the “target” qubit.

For semiconductors with zinc blende structures ( such as, Si and GaAs *etc.* ), spin polarization of conduction electrons in semiconductors can be produced by near-infrared laser light with circularly polarized light working at the band gap [32]. Since electron and nuclear spins are coupled by the hyperfine interaction, polarization is transferred between electrons and nuclei by the spin flip-flop transitions. Through many optical pumping cycles, large polarization of nuclear spins can be achieved at low temperature. When the large nuclear spin polarizations are produced, one can directly detect NMR signals from hyperpolarized nuclei in the semiconductors with conventional NMR techniques or optical techniques.

In addition, since optical detection of NMR is extremely sensitive, which can detect NMR signals from fewer than  $10^4$  [39] nuclei, the optical methods are naturally preferable to the conventional NMR methods. Optical detection is mainly based on the following two mechanisms. In direct-gap semiconductors, a conduction electron can emit a circularly polarized photon through recombining with a hole in the hole band. The degree of circular polarization of the photoluminescence depends on the polarization of the conduction electrons. The hyperfine interaction leads to spin polarization transfer between electrons and nuclei. Therefore it is possible to detect NMR in direct-gap semiconductors indirectly by optical detection methods [32]. In addition, under NMR conditions, hyperpolarized nuclei in semiconductors can act back on electron spins by the hyperfine interaction so that they shift electron Zeeman levels ( Overhauser shift ) [39] and change polarization of electron spins. This is because hyperpolarized nuclei exert a magnetic field ( called the nuclear hyperfine field ) on the electron spins [39]. The nuclear hyperfine field is directly proportional to the nuclear spin polarization. Radio-frequency pulse near an NMR transition can change the strength and direction of this field. The net magnetic field felt by the electron spins depends on the combined action of this field and the externally applied magnetic field. The shift of the conduction electron Zeeman levels results from the change of the net magnetic field. It is possible to measure this Overhauser shift [39] and the polarization of the photoluminescence through sensitive optical spectroscopies with tunable lasers and highly sensitive detectors under NMR conditions [39]. Therefore one indirectly measures NMR in the direct-gap semiconductors by optical detection methods.

In the following, we shall discuss how to prepare and measure the states of the nuclear spins in the direct-gap semiconductors and how to perform the controlled rotation operation on the nuclear spins in our scheme.

For simplicity, we shall take the direct-gap semiconductor InP into account, which has electronic levels similar to GaAs ( see Fig. 2a ) [32]. Near the  $\Gamma$  point ( electronic Bloch wavevector  $k$  is equal to zero ), an excess of conduction electrons with  $m_{1/2} = +1/2$  can be produced by using circularly polarized light with helicity  $\sigma^-$  tuned to the band gap (  $E_g \approx 1.42eV$  in InP near 0 K ) [32]. The direction of the conduction electron spin polarization can be controlled by circularly polarized light with different helicities ( such as  $\sigma^-$  or  $\sigma^+$  ). Electron spin polarization can be transferred to the  $^{31}P$  nucleus by the hyperfine interaction. In addition, the  $^{31}P$  nuclear resonance frequency change is directly proportional to the electron spin polarization  $\langle S_z \rangle$  [40], i.e.  $\Delta f = A\rho(z')\langle S_z \rangle$  [40], where  $A$  is a coupling constant,  $\rho(z')$  is the conduction electron density envelop function,  $z'$  is the displacement of nucleus from a conduction electron and  $\langle S_z \rangle$  is electron spin polarization. The nuclear resonance frequency of  $^{31}P$  can be written as:  $\nu = \gamma B_0/2\pi + \Delta f$ , where  $\gamma$  is the gyromagnetic ratio and  $B_0$  is the externally applied magnetic field. Therefore one can use the observed NMR frequency shift based on positive or negative electron spin polarization  $\langle S_z \rangle$  to control  $^{31}P$  nuclear rotations by using selective r.f. pulses. For example, only when the electron spin polarization is positive, a radio pulse required to flip spin can be used to selectively change the states of the nucleus. When the electron spin polarization is negative, one has no use for doing anything. Therefore, one can perform the controlled rotation operations of  $^{31}P$  nuclear spin on the basis of different directions of electron spin polarizations.

The purpose of optical pumping in the computer is to control the hyperfine interaction between electrons and nuclei, indirectly to mediate nuclear spin interactions, to produce electron and nuclear spin polarization and indirectly to measure nuclear spin polarization. For example, when the valence band electrons are excited to the conduction band near the  $\Gamma$  point, the large hyperfine interaction energy is yielded. This is because near the  $\Gamma$  point, the conduction band is primarily composed of wavefunctions with  $s$  orbits so that the electron wavefunctions are concentrated at the nucleus. When one uses a laser to pump a cell between two cells in the semiconductors (see Fig. 2b ), it can enhance nuclear dipole-dipole interactions and mediate the indirect nuclear spin coupling. This is because when the electrons are excited to the conduction band by a laser, the conduction electron wavefunction ex-

tends over large distance through the crystal lattice and large electron spin polarizations are produced. Electron spin polarization can be transferred to nuclear spins by the hyperfine interaction. As soon as larger nuclear spin polarizations are produced, the nuclear spins act back on the electron and shift the electron Zeeman energy ( Overhauser shift ) [39]. By measuring the magnitude of the Overhauser shift under NMR conditions, it is possible to measure the states of nuclei with the Raman spectroscopy [39].

On the basis of the above discussions, in the following, we shall discuss how to prepare the cell magnetization in an initial state, how to perform the controlled rotation operations of  $^{31}\text{P}$  nuclear spin, how to couple the effective pure states of the two adjacent cells and how to measure the effective states of logic gates at different cells.

Optical pumping in the computer can be used to prepare the electron spin states and the nuclear spin states, i.e. control qubits and target qubits. As we have seen, one can pump the electrons in valence band into positive or negative polarizations of conduction electrons by using circularly light with different helicities (  $\sigma^-$  or  $\sigma^+$  ). Therefore an initial state in a cell can be loaded with circularly polarized light with different helicities (  $\sigma^+$  or  $\sigma^-$  ). For example, in order to prepare electron and nuclear spins up ( at a magnetic field ), spin up of the conduction electrons can be produced with circularly polarized light with helicity of  $\sigma^-$  tuned to the band gap, and spin up of  $^{31}\text{P}$  nuclei can also be prepared by the hyperfine interaction. Similarly, one can prepare electron and nuclear spins down with circularly polarized light with helicity of  $\sigma^+$  . In Fig.2b, one uses many laser beams with different helicities (  $\sigma^+$  or  $\sigma^-$  ) to initial logic gates at different cells in the different states.

The controlled rotation operations of  $^{31}\text{P}$  nuclear spins can be performed by r.f pulses with different frequencies on the basis of the states ( spins up or down ) of the conduction electrons at different cells, as has been discussed above.

In Fig.2b, entanglements of effective pure states between cell 1 and cell 3, might be performed by the following means. Between two logic gates ( such as 1 and 3 in Fig.2b ), if one uses laser with higher power to pump cell 2, one can produce much more conduction electrons near cell 2 and obtain higher polarization of the conduction electrons at cell 2, laser pumping at cell 2 results in the electron wavefunction at the cell extending over large distances through the crystal lattice. The electron spin dipole-dipole interactions between these two gates ( 1 and 3 ) are increased through the conduction electrons of the 2 cell mediating electron spin dipole-dipole inter-

actions between cell 2 and cell 1, and cell 2 and cell 3. Therefore one can use pumping laser light indirectly to mediate an indirect coupling between  $^{31}\text{P}$  qubits of two cells by means of the  $^{31}\text{P}$  electron-nuclear hyperfine interaction. If one uses pumping laser with low or no power to pump cell 2, one can decrease the indirect interactions between  $^{31}\text{P}$  qubits of two cells so that two gates 1 and 3 can independently work. As the distance between two cells is increased, the interactions between distant logic spin will no longer be effective, Fortunately, universal quantum computation is still possible with just local interactions [31] [45]. This is because one can use a cellular automata architecture to perform any function computations in a linearly-increasing computational time with system size due to message passing [45] .

The  $^{31}\text{P}$  nuclear spin states at a cell can indirectly be measured with the Raman spectroscopy [39]. This is because when  $^{31}\text{P}$  nuclear spin is up or down, the magnitude of the Overhauser shift under NMR conditions is different [39].

Can we construct different logic gates in space in semiconductor? i.e. can one make logic gates addressable? In Fig.2b, similar to the scheme of trapped ion quantum computer [18] , we use N different laser beams with different helicities to pump and detect different cells in space in the InP semiconductor, together with the externally applied gradient magnetic fields and r.f. gradient pulses, so that we can build up any logic gates in space.

## 4 Conclusion

We have described the two schemes for implementing the controlled NOT gates in NMR quantum computers. It is possible to realize these two proposals with current techniques. Optical pumping in solid state NMR can circumvent the two problems of relatively low sensitivity and lack of spatial selectivity in solid state NMR. Therefore it is possible to construct quantum logic gates in space. The schemes could be useful for implementing actual quantum computers in terms of a cellular automata architecture. It should be noted that nuclear spin polarization in optical pumping solid state NMR does not depend on the strength of magnetic fields. The experiments can be performed in low fields produced by the general electromagnets or the magneto irons. The experimental demonstration of our proposal with optical pumping in solid state NMR and modern NMR techniques is possible.

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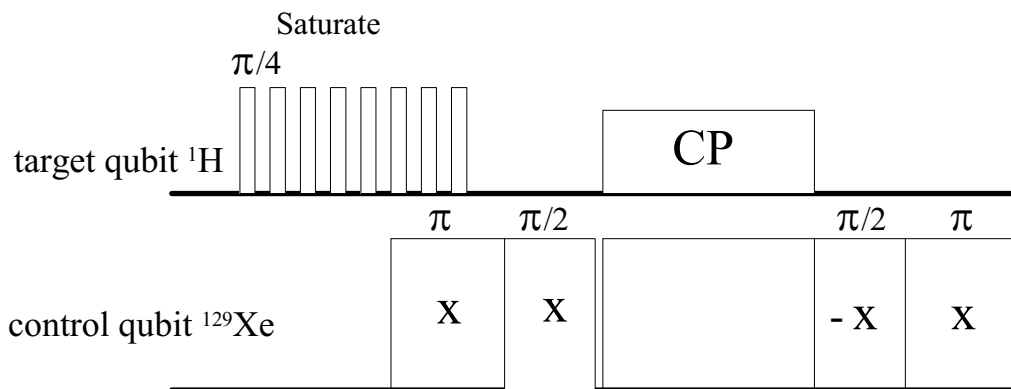
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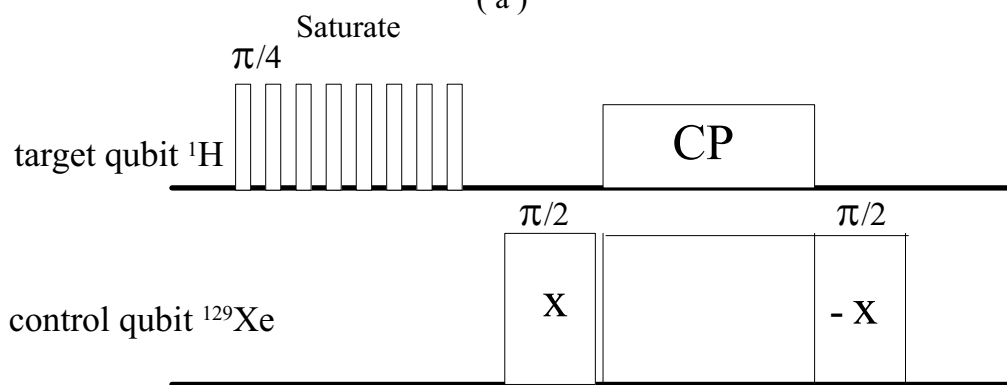
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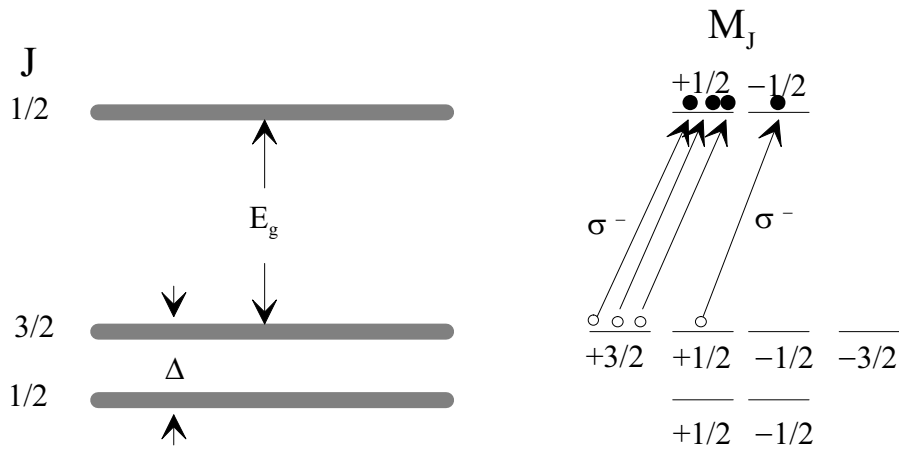
( a )



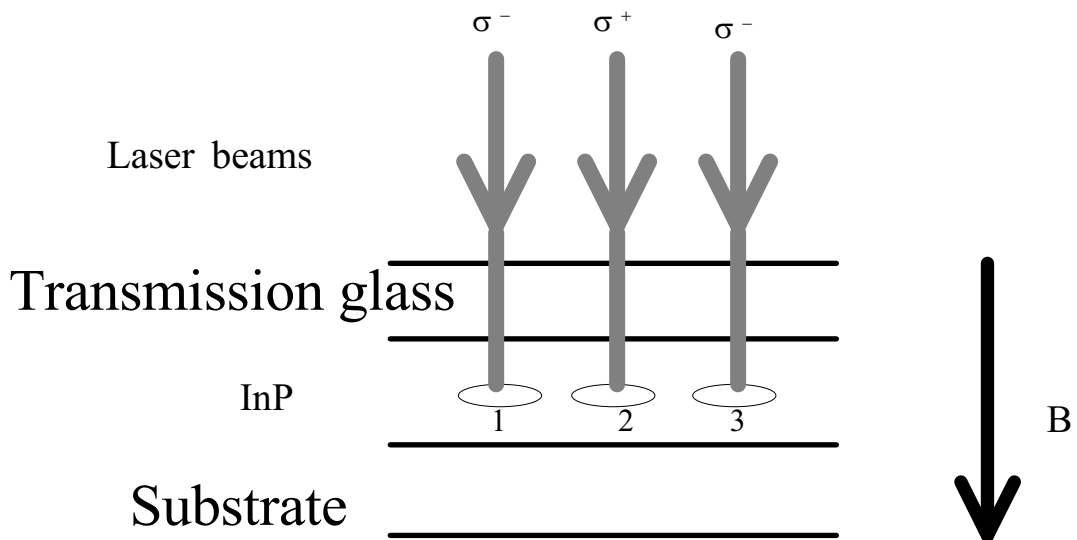
( b )

Fig.1. NMR pulse sequences for realization of the CNOT gate.  
 (a) Corresponding to the target qubit ( $^1\text{H}$ ) initially existing in the  $|1\rangle$  state.  
 (b) Corresponding to the target qubit ( $^1\text{H}$ ) initially existing in the  $|0\rangle$  state.





(a)



(b)

Fig. 2. (a) Energy levels and transitions of electron systems relative to our schemes in the InP semiconductor.

(b) Three cells in the InP semiconductor pumped with three different laser beams.