Nuclear-spin qubits interaction in mesoscopic wires
and rings

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Abstract. Theoretical study of the indirect coupling of nuclear spins (qubits) embedded into a mesoscopic ring and in a finite length quantum wire in a magnetic field is presented. It is found that the hyperfine interaction, via the conduction electrons, between nuclear spins exhibits sharp maxima as function of the magnetic field and nuclear spin positions. This phenomenon can be used for manipulation of qubits with almost atomic precision. Experimental feasibility and implications for quantum logics devices is discussed.

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Introduction

The possibility that a computer could be built employing the laws of quantum mechanics has stimulated huge interest in searching for useful algorithms and realizable physical implementations [1]. There are currently many promising approaches to quantum computation [2], the most promising solid state approaches are based on the superconductivity [3], conduction electron spins [4] and nuclear spins [5, 6, 7, 8, 9, 10] as qubits. The attraction of the approach of using nuclear spin in quantum computation lies in the idea of incorporating nuclear spins into a semiconductor device [5, 6, 7]. Using of the nuclear spins incorporated in a heterostructure in the highly nondissipative quantum Hall effect regime, as qubits [5], are promising because they are extremely well isolated from their environment and have a long decoherence time [11, 12, 13]. The energy gap in the spectrum of two-dimensional electrons in a strong magnetic field imposes severe restriction on the flip-flop processes, since the electron Zeeman energy is orders of magnitude larger than the nuclear one [13]. It follows that the nuclear
spin imbedded in 2DES under the QHE conditions is practically decoupled from the conduction electron spins. As a result the nuclear spin relaxation time has an activation behavior, i.e. is exponential in the electron energy gap and inverse temperature \cite{13} and can be manipulated by external magnetic field and sample parameters over several orders of magnitude time interval.

A set of five essential criteria for the physical realization of a quantum computer was formulated by DiVincenzo and coworkers \cite{14}. They are:

1. A scalable physical system with well characterized qubits. The system should consist of a collection of independent subsystems each with a two-dimensional Hilbert space, so-called quantum bits, or qubits. Its physical parameters should be accurately known, including the internal Hamiltonian of the qubit, the presence of and couplings to other states of the qubit, the interactions with other qubits, and the couplings to external fields that might be used to manipulate the state of the qubit.

2. The ability to initialize the state of the qubits to an initial state. This arises from computing requirement that registers should be initialized to a known value before the start of computation. Moreover, the initialization of qubits is used in quantum error correction algorithms.

3. Long relevant decoherence times, much longer than the gate operation time. It was shown that for fault-tolerant quantum computation the magnitude of decoherence time scales should be $10^4 - 10^5$ times the "clock time" of the quantum computer, that is, the time for the execution of an individual quantum gate.

4. A `universal’ set of quantum gates. a) It should be possible to perform precise unitary operations on the individual qubits. b) Furthermore, the inter-qubit interaction should be controlled with almost atomic precision.

5. A qubit-specific measurements capability. Any quantum computer would deliver its output as results of measurements performed on it.

In what follows we concentrate on nuclear spin based solid state models \cite{5, 6, 7, 11, 8, 12, 9}. All the existing models satisfy the criteria 1,2 and 4a. In some models the criteria 3 is almost satisfied. At least, the ratio of gate to decoherence time allows to create a few qubit quantum computer. No existing model addresses the problem of controlling the inter-qubit interaction with atomic precision. In this paper we propose a new system in which criteria 1-4 are completely fulfilled. Our investigation is mainly focused on the criterion 4b.

The proposed system consists of nuclear spins (qubits) embedded into a zero nuclear spin mesoscopic ring or a finite length quantum wire (Fig. 1a and Fig. 2a). The hyperfine interaction of the electrons in the system with nuclear spins leads to an effective indirect nuclear spin interaction. In what follows we calculate the effective nuclear spin interaction energy. The effective nuclear spin interaction energy can be chosen to have the following form:

$$E = (I_{1,x}I_{2,x} + I_{1,y}I_{2,y})A + I_{1,z}I_{2,z}B,$$

where $\mathbf{I}_i$ is magnetic moment of a nucleus, $A$ and $B$ are functions of the system
parameters as described below. We obtain that the effective nuclear spins interaction exhibits sharp maxima as function of the magnetic field and nuclear spin positions which opens the way to manipulate qubits with almost atomic precision. The selective nuclear spin interaction can be obtained by changing external parameters of the system.

The first calculation of the indirect, via electron spins, hyperfine coupling between nuclear spins, was performed by Ruderman and Kittel [15] for the case of 3D metal in the absence of magnetic field (see [16]). Influence of mesoscopic effects on the RKKY interaction was studied by Spivak and Zyuzin [17]. They pointed out that the only difference between pure and impure metals is an additional random phase which depends on impurity distribution. A mechanism of the indirect, via the exchange of virtual electron-hole pairs (spin excitons), nuclear spin interaction in the quantum Hall effect systems was suggested in [18] and further elaborated in [8]. Quantum computation and communication devices, based on this mechanism are proposed in [5, 8, 9].

Theoretical framework and results

Let us consider a system consisting of electrons confined by a potential $V(r)$ and interacting with two nuclear spins. We assume that the nuclear spins are located far enough from each other, so that the direct (dipole-dipole) nuclear spin interaction is negligibly small as is in isotopically engineered Si/Ge heterojunctions [9]. The contact hyperfine interaction between electrons and nuclear spins leads to an indirect nuclear spin interaction.

The wave function of the electron $\phi(r)$ can be written as a product of an envelope function $\Psi(r)$ by the rapidly varying periodic function $u'_0(r)$ [19]

$$\phi(r) = \Psi(r)u'_0(r) = \Psi(r)u_0(r)(V/\Omega)^{\frac{1}{2}}$$

where $u_0(r)$ is the $k = 0$ Bloch state, $V$ is the volume of the sample, and $\Omega$ is the volume of the unit cell. The function $u'_0(r)$ is conveniently normalized in the cell volume $\Omega$,

$$\int_{\Omega} |u'_0(r)|^2 \, dr = 1.$$  

The localization of electrons is described by the envelope part of the wave function $\Psi(r)$. The norm of the envelope function is

$$\int_{V} |\Psi(r)|^2 \, dr = \Omega$$.

In what follows we will consider the system in the envelope function approximation, the rapidly varying function $u'_0(r)$ appears only in the expression for hyperfine interaction. The Hamiltonian of the system is given by $H = H_0 + H_1^{(1)} + H_1^{(2)}$ with

$$H_0 = \frac{1}{2m^*} \left( p + eA \right)^2 + V(r) - g\mu_B \sigma \mathbf{H}$$

and

$$H_1^{(i)} = \frac{8\pi}{3} \mu_B \hbar \gamma_n |u'_0(r_i)|^2 \sigma I_i \delta(r - r_i)$$

where $H_0$ is the Hamiltonian of the electron in the mesoscopic structure in the magnetic field, $H_1^{(1)} + H_1^{(2)}$ is the perturbation due to the contact hyperfine interaction, $m^*$ is the effective electron mass, $A$ is the vector-potential, $g$ is the electron $g$-factor, $\mu_B$ is the
Bohr magneton, $\mathbf{H}$ is the magnetic field, $\gamma_n$ is the nuclear gyromagnetic ratio, $\mathbf{I}$, and $\sigma$ are nuclear and electron spins, $\mathbf{r}_i$ is radius vector of $i$ nucleus, $i = 1, 2$. Because the electron wave function is strongly peaked on the nuclei, the contact hyperfine interaction energy greatly exceeds dipolar spin interactions.

The effective nuclear spin interaction energy calculated in a second-order perturbation method is given by the expression $[16]$

$$E = \sum_{E_i, E_f} \frac{\langle \Psi_i | H^{(1)}_i | \Psi_f \rangle \langle \Psi_f | H^{(2)}_i | \Psi_i \rangle}{E_f - E_i} f_i (1 - f_f) + c.c. \quad (5)$$

Here $\Psi_i$ and $E_i$ are eigenfunctions and eigenvalues of $H_0$ and $f_i$ is the electron distribution function. In this Letter we restrict ourselves to the single electron approximation, which proved to be sufficient for clean low density quantum wires and rings, see $[20]$ and references therein. Presence of impurities violates the Kohn theorem $[21]$ and the electron interactions may play an important role. In strongly correlated dense 1D electron systems the Fermi liquid approach should be replaced by the Tomonaga-Luttinger theory, see $[22]$ and references therein. The influence of the electron correlations on the results obtained here will be the subject of a more detailed publication.

Nuclear-spin interaction in mesoscopic rings

Consider a torus-shaped quantum ring of inner radius $a$, thickness $d \ll a$ and negligible height $h$ $[23]$ in a uniform parallel to the axis of the ring magnetic field $\mathbf{H}$ in $z$ direction with two nuclear spins located at $\mathbf{r}(\rho, \varphi, z) = \mathbf{r}_1 (a + d/2, \varphi_1, h/2)$ and $\mathbf{r} = \mathbf{r}_2 (a + d/2, \varphi_2, h/2)$ (Fig.1a). In this subsection we use the polar coordinates. The electron confining potential $V(\rho, z)$ is

$$V(\rho, z) = \begin{cases} 0 & \text{if } a \leq \rho \leq a + d \text{ and } 0 \leq z \leq h, \\ \infty & \text{otherwise}. \end{cases} \quad (6)$$

Firstly, let us find eigenfunctions and eigenvalues of the Shr"odinger equation with the Hamiltonian $[3]$. Due to the axial symmetry of the ring, the wave function can be written as follows

$$\Psi_{m,n,s=\pm} = \sqrt{\frac{\Omega}{2\pi}} \left( \begin{array}{c} 1 \\ 0 \end{array} \right) e^{im\varphi} R_{m,n}(\rho) Z_1(z) \quad (7)$$

We assume that in $z$ direction the electron is always on the ground level of the one-dimensional quantum well of thickness $h$, thus $Z_1(z) = \sqrt{\frac{2}{h}} \sin \left( \frac{\pi z}{h} \right)$. Over the region $a \leq \rho \leq a + d$ the radial part of the wave function $R_{m,n}(\rho)$ satisfies the equation:

$$-\frac{\hbar^2}{2m} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} R_{m,n} + \frac{\hbar^2}{2m_e\rho^2} \left( m + \frac{\Phi(\rho)}{\Phi_0} \right)^2 R_{m,n} = E_{m,n} R_{m,n}. \quad (8)$$
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where \( \Phi_0 \) is the magnetic flux quantum and the radial number \( n = 1, 2, 3, \ldots \). The boundary conditions imposed by the potential \( V(\rho, z) \) are: \( R_{m,n}(a) = 0 \) and \( R_{m,n}(a + d) = 0 \).

We will look for the solution of Eq. (8) assuming that at \( d \ll a \) the vector-potential varies slow in the ring, so we can put \( \Phi(\rho) \simeq \Phi(a + d/2) \). In this case the solution of Eq. (8) is written in terms of Bessel functions:

\[
R_{m,n}(\rho) = C_1 J_A(\rho \alpha_{m,n}) + C_2 Y_A(\rho \alpha_{m,n}) \tag{9}
\]

where \( A = \left| m + \frac{\Phi(a+d/2)}{\Phi_0} \right| \) and \( \alpha_{m,n} = \sqrt{\frac{2m_n E_{m,n}}{\hbar^2}} \), the constants \( C_1, C_2 \), energy levels \( E_{m,n} \) are defined by boundary conditions and the normalization condition

\[
\int_a^{a+d} \rho R_{m,n}(\rho) R_{m,n}(\rho) d\rho = 1. \tag{10}
\]

Unfortunately, the wave function of the form (9) allows to calculate the effective nuclear spin interaction only numerically.

To obtain an analytical result, consider the effective interaction energy constants \( A \) and \( B \) for the case of infinitely narrow ring. To do this, let us set \( \rho = a \) in (8). It is readily seen that in this case the radial part of wave function decouples from the orbital part, \( R_n(\rho) = \sqrt{\frac{\pi}{d}} \sin \left( \frac{(\rho-a)\pi}{d} \right) \) and

\[
E_{n,m,s=\pm} = \frac{\hbar^2}{2m^*} \left( \frac{\pi n}{d} \right)^2 + \frac{\hbar^2}{2m^* a^2} \left( m + \frac{\Phi(a+d/2)}{\Phi_0} \right)^2 \mp g\mu_B H/2. \tag{11}
\]

For the infinitely narrow ring it’s reasonable to consider the states only with \( n = 1 \). With Eq. (11), the effective nuclear spin interaction constants are:

\[
A = K_r \sum_{m,n} \frac{\cos((n-m)(\varphi_1 - \varphi_2))}{E_{1,n,+} - E_{1,m,-}} f(E_{1,m,-})(1 - f(E_{1,n,+})) \tag{11}
\]

\[
B = K_r \sum_{m\neq n} \frac{\cos((n-m)(\varphi_1 - \varphi_2))}{E_{1,n,+} - E_{1,m,+}} f(E_{1,m,+})(1 - f(E_{1,n,+})) \tag{12}
\]

where \( K_r = 2 \left( \frac{16}{\pi d^2 n^2} \Omega \mu_B \hbar \gamma_n |\psi_n(0)|^2 \right)^2 \).

Using the wave function in the form Eq. (7), we numerically calculate the magnetic field dependencies of the nuclear spin interaction constants \( A \) and \( B \) using the following set of parameters: \( \varphi_1 = 0, \varphi_2 = \pi, a = 100 nm, h = 1nm, d = 1nm \) and \( 0.5nm \), one electron in the ring, \( T = 0 \). The results of our calculations are shown on Fig.1b. The magnetic field dependence of the effective nuclear spin interaction constants are defined by the energy level statistics. The nuclear spin interaction constant \( A \) describes nuclear spin flip-flop processes which are performed through flips of electron spin, and, therefore, the main contribution to this process is due to the energy levels with the same orbital quantum numbers and different spin directions, what gives \( 1/H \) dependence of the interaction amplitude. The nuclear spin coupling constant \( B \) is connected with electron transitions between energy levels with different orbital quantum numbers, but the same electron spin direction. Their periodicity with the magnetic field results in the periodicity of the constant \( B \). It is seen that at the values of the magnetic field, when
there are two ground states, function $B$ has discontinuities. In this case the perturbation theory is not applicable. The obtained result is in a good agreement with the result obtained for the case of infinitely narrow ring potential Eqs.\cite{11, 12}.

**Nuclear-spin interaction in mesoscopic wires**

The next system under consideration is a finite length quantum wire of the length $l$ in $x$-direction, of the thickness $d$ and of the height $h$ with two nuclear spins located at $r(x, y, z) = r_1(l_1, d/2, h/2)$ and $r = r_2(l_2, d/2, h/2)$ in a magnetic field $H$ in $z$ direction (Fig. 2a). We suppose that the transversal sizes of quantum wire are much smaller than the length of the quantum wire and the cyclotron orbit of electron. We consider a model, when the confining potential is

\[
V(x) = \begin{cases} 
0 & \text{if } 0 \leq x \leq l, 0 \leq y \leq d, 0 \leq z \leq h \\
\infty & \text{otherwise.}
\end{cases}
\]  

The eigenfunctions and eigenvalues of the Hamiltonian (3) with potential (13) are

\[
\Psi_{n,m,k,\pm} = \sqrt{\frac{8}{ldh}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} n\pi x/l \\ m\pi y/d \\ k\pi z/h \end{pmatrix}, \quad E_{n,m,k,\pm} = \frac{\hbar^2 \pi^2}{2m^*l^2} n^2 + \frac{\hbar^2 \pi^2}{2m^*d^2} m^2 + \frac{\hbar^2 \pi^2}{2m^*h^2} k^2 \mp g\mu_B H/2, \]  

As in the case of the nuclear spin interaction in mesoscopic wires, we assume that $d, h \ll l$, so we consider only the electrons on the ground levels of potential wells in $y$ and $z$ directions, i.e. $m = k = 1$. Substitution of Eqs. (14) and (15) into (5) gives us the effective nuclear spin interaction constants.

We have calculated analytically and numerically the effective interaction constants $A$ and $B$ as a functions of nuclear spin positions for odd and even number of electrons $N$ in the wire. The results of calculation for the odd number of electrons ($N = 9$) at $T = 0$ are presented at Figures 2b-2d. In low magnetic field region, when Zeeman splitting energy is much less than the energy gap between levels with different $n$ (Eq.(15)) and at $T = 0$ limit the expression for $A$ takes a simple form:

\[
A = Kw \left( \frac{\sin \left( \frac{(N+1)\pi l_1}{2l} \right) \sin \left( \frac{(N+1)\pi l_2}{2l} \right)}{g\mu_B H} \right)^2,
\]  

where $Kw = 2 \left( \frac{64\pi\Omega_B \hbar \gamma_n |u'_0(0)|^2}{3ldh} \right)^2$. In this limit the interaction constant $A$ has a set of $\frac{(N+1)^2}{4}$ maximums (Fig. 2b) and $B \ll A$. Fig. 2c shows an increasing of interaction constant $A$ if nuclear spins are located not far from each other (in the vicinity of the line $l_1 = l_2$) and a decreasing of interaction constant $A$ for the other nuclear spin positions with increasing of the magnetic field. The interaction constant $B$ has a non-trivial dependence on the nuclear spin positions (Fig. 2d).
Conclusions and discussion

To conclude, we proposed a new possible implementation of a basic unit for quantum computer based on the nuclear-spin qubits embedded into the zero nuclear spin mesoscopic ring or finite length quantum wire. Particular emphasis has been placed on the investigation of nuclear spin interaction via the electrons confined in such systems. It was found that the indirect nuclear-spin qubit interaction is very sensitive to the system parameters: nuclear spin location, number of electrons, magnetic field and geometry of the system. Its dependence on the system parameters is completely different from indirect nuclear spin interaction in 2D and 3D metals. Preliminary finite temperature calculation indicates that the values of the effective nuclear spin interaction constants are decreasing with temperature, but the main features of the obtained results remain qualitatively unchanged.

Now let us consider how our model of quantum computer is matched by the set of DiVincenzo criteria listed in the Introduction.

1. It’s well known that nuclear spins are appropriate candidates to be qubits [6, 10]. Nuclei with spin $1/2$ are two-level systems with well defined states $|0>$ and $|1>$. Needless to say that such a system is scalable and, basically, there is no principal limitation on the reasonable number of nuclear-spin qubits which can be integrated into a quantum circuit. The ring architecture of the quantum computer is of considerable promise. Let us imagine a mesoscopic ring with nuclear-spin qubits located in the immediate vicinity of it. A local change of the electrostatic potential near a qubit by a gate electrode changes the value of the envelope wave function on the qubit and, correspondingly, allows to switch on the interaction between any two qubits, whereas almost at all quantum computer proposal only adjacent qubits can directly interact. Nuclear-spin qubit interaction through electrons confined on a sphere opens a further way to improve the quantum computer architecture.

2. We propose to initialize the nuclear-spin qubits using spin-polarized electrons. There is a general agreement that it is the only feasible method since the nuclear spins are highly isolated from the environment. Possibility of nuclear spin polarization by spin-polarized transport was demonstrated almost ten years ago [24, 25]. Possible methods to introduce nonequilibrium polarizations of the electrons include injections of spins from ferromagnetic contacts [26], optical pumping [27, 28] and spin refrigeration (see [7] and references therein).

3. The decoherence time of the nuclear spins in mesoscopic systems is expected to be long enough to perform the quantum computation, since the discrete electron spectrum in mesoscopic systems imposes restriction on the flip-flop processes and the nuclear spin relaxation time at low temperatures is expected to have an activation behavior [13]. Up to the present, a calculation of nuclear spin decoherence time in mesoscopic structures is not made, however as a rough estimation we can take the decoherence time of the nuclear-spin qubit embedded into 2DEG, $T_2 = 10$ sec [10]. The characteristic time of qubit interaction is $T_{int} \sim h/A$, where for the nuclear-spin qubits
in finite length quantum wire $A$ is given by Eq. (16). Using available experimental data for GaAs, $|u_0'(0)|^2_{\gamma, As} = 9.8 \cdot 10^{25} \text{cm}^{-3}$ [19] and following set of parameters: $a = 200nm$, $d = h = 5nm$, $H = 0.01T$ we obtain $T_{\text{int}} = 2 \cdot 10^{-5} \text{sec}$ and $T_2/T_{\text{int}} = 5 \cdot 10^5$. Our estimate indicates that the present system is suitable for fault-tolerant quantum computation.

4. a) The one-qubit operations using the NMR could be similar to the existing experimental suggestions [5, 8, 9]. b) Interaction between any two qubits, which is necessary for two-qubit operations, is performed by the confined electrons. By varying the external parameters (magnetic field, number of electrons, gate potentials) we can control with almost atomic precision the nuclear spin interaction strength by creating maxima of the amplitude of electron wave function on some qubits and zero on the other. As an example, consider how it is possible to control nuclear-spin qubit interaction in the finite length wire by changing the number of electrons. Let us place the qubits at some predefined positions with coordinates $x_i = \frac{\alpha_i}{\beta_i}$, where $\beta_i$ are different prime numbers and $\alpha_i$ are integers ($\alpha_i < \beta_i$). The orbital part of the last electron level wave function (from Eq. (14)) for

$$ N_{jk} = 2 \prod_{i=1}^{M} \frac{\beta_i}{\beta_j \beta_k} - 1, \quad (17) $$

electrons in the system is

$$ \Psi_{n,m,k,\pm} = \sqrt{\frac{8}{ldh}} \sin \left( \frac{\pi}{l} \prod_{i=1}^{M} \frac{\beta_i}{\beta_j \beta_k} x \right) \sin \left( \frac{m\pi y}{d} \right) \sin \left( \frac{k\pi z}{h} \right). \quad (18) $$

It is readily seen that $\Psi_{n,m,k,\pm}(x_i) = 0$ for $i \neq j, k$. This means, that all qubits except $j$ and $k$ are at the nodes of the wave function and only $j$ and $k$ qubits interact. Fig. 3 illustrates this idea. It follows that the accuracy of nuclear spin positioning should be few atomic units.

5. In mesoscopic systems the single nuclear-spin measurement is still an open problem. One of the possibilities is to use Hyperfine Aharonov-Bohm effect (HABE) [29], following from the coupling of the nuclear spin polarization to the phase of the conduction electron wave function. This was outlined in [5] and will be considered in details elsewhere. Another possibility is to use spin-dependent magneto-transport tunneling through a system, which energy levels are spin-split by an external magnetic field [30]. The tunneling current develops a distinctive peak at the frequency of Zeeman splitting, which can be sufficiently narrow to measure a state of the nuclear spin. Moreover, it’s possible to use spin to charge conversion as it was discussed in [7].

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Figure 1. a) Two nuclear spins embedded into a torus shaped quantum ring; b) dependence of nuclear spin coupling constants $A$ and $B$ on the magnetic field, $E_r = \frac{h^2}{2m^* a^2}$. 
Figure 2. a) Two nuclear spins embedded into a finite length quantum wire in a magnetic field; b) nuclear spin coupling constant $A$ in low magnetic field region \(\frac{\hbar\mu_B e^2 H}{\hbar^2} = 0.1\); c) nuclear spin coupling constant $A$ in high magnetic field region \(\frac{\hbar\mu_B e^2 H}{\hbar^2} = 3\) and d) nuclear spin coupling constant $B$ on the nuclear spin positions. Odd number of electrons, $T = 0$, the nuclear spin coupling constants are given in units of $K_w/E_w$, where $E_w = \frac{\hbar^2 e^2}{2m^* l^2}$. 
Figure 3. Qubit arrangement and the last occupied electron level wave function for $N = 3, 5, 9$ electrons in the wire. The qubits are located in the nodes of the different wave functions.