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Indirect hyperfine interaction between nuclear spin qubits in mesoscopic wires and rings

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Abstract

A theoretical study of the indirect coupling of nuclear spins (qubits) embedded in 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 a 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 logic devices is discussed.

(Some figures in this article are in colour only in the electronic version)

1. 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 superconductivity [3], conduction electron spins [4], and nuclear spins [5–10] as qubits. The attraction of the approach of using nuclear spins in quantum computation lies in the idea of incorporating nuclear spins into a semiconductor device [5–7]. Using the nuclear spins incorporated in a heterostructure in the highly non-dissipative quantum Hall effect regime as qubits [5] is promising because they are extremely well isolated from their environment and have a long decoherence time [11–13]. The energy gap in the spectrum of two-dimensional electrons in a strong magnetic field imposes severe restrictions 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 embedded in a 2DES under QHE conditions is practically decoupled from the conduction electron spins. As a result the nuclear spin relaxation time has an activation behaviour, i.e. is exponential in

the electron energy gap and inverse temperature [13], and can be manipulated by an external magnetic field and sample parameters over a time interval of several orders of magnitude.

A set of five essential criteria for the physical realization of a quantum computer was formulated by DiVincenzo and co-workers [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 the 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 the decoherence timescales 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 measurement 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 [5–9, 11, 12]. All the existing models satisfy the criteria (1), (2), and (4a). In some models the criterion (3) is almost satisfied. At least, the ratio of gate to decoherence time allows one 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 in a zero-nuclear-spin mesoscopic ring or a finite-length quantum wire (figures 1(a) and 2(a)). 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:

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

where $\boldsymbol{I}_i$ is the magnetic moment of a nucleus, and A and B are functions of the system parameters as described below. We find that the effective nuclear spin interaction exhibits sharp maxima as a function of the magnetic field and nuclear spin positions, which opens the way to manipulating qubits with almost atomic precision. The selective nuclear spin interaction can be obtained by changing the 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 a magnetic field (see [16]). The 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 the 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

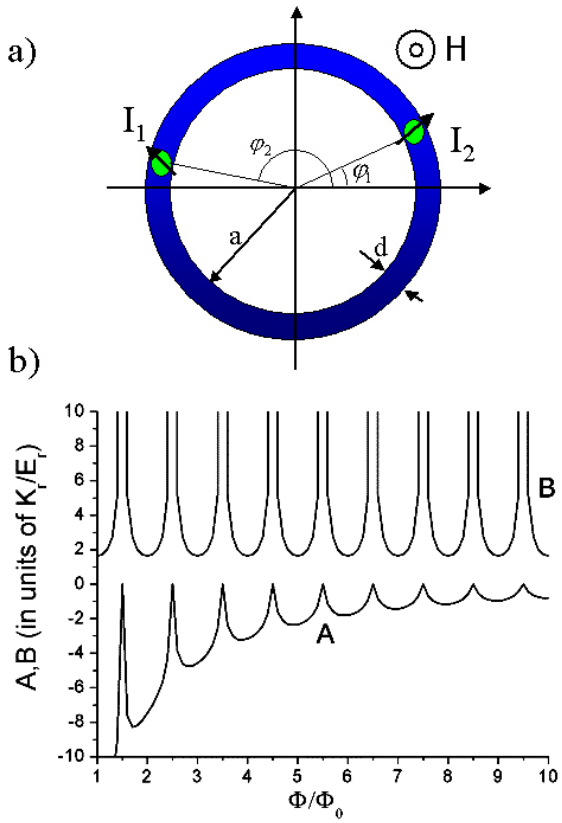

Figure 1. (a) Two nuclear spins embedded in a torus-shaped quantum ring; (b) the dependence of the nuclear spin coupling constants A and B on the magnetic field, $E_r = \frac{\hbar^2}{2m^*a^2}$.

elaborated in [8]. Quantum computation and communication devices based on this mechanism are proposed in [5, 8, 9]

2. Theoretical framework and results

Let us consider a system consisting of electrons confined by a potential $V(\boldsymbol{r})$ and interacting with two nuclear spins. We assume that the nuclear spins are located far enough from each other that the direct (dipole–dipole) nuclear spin interaction is negligibly small as it 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 wavefunction of the electron $\phi(\boldsymbol{r})$ can be written as a product of an envelope function $\Psi(\boldsymbol{r})$ with the rapidly varying periodic function $u_0'(\boldsymbol{r})$ [19]:

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

where $u_0(\boldsymbol{r})$ is the $\boldsymbol{k} = 0$ Bloch state, V is the volume of the sample, and Ω is the volume of the unit cell. The function $u_0'(\boldsymbol{r})$ is conveniently normalized in the cell volume Ω, $\int_\Omega |u_0'(\boldsymbol{r})|^2 \,\mathrm{d}\boldsymbol{r} = 1$. The localization of electrons is described by the envelope part of the wavefunction $\Psi(\boldsymbol{r})$. The norm of the envelope function is $\int_V |\Psi(\boldsymbol{r})|^2 \,\mathrm{d}\boldsymbol{r} = \Omega$ [19].

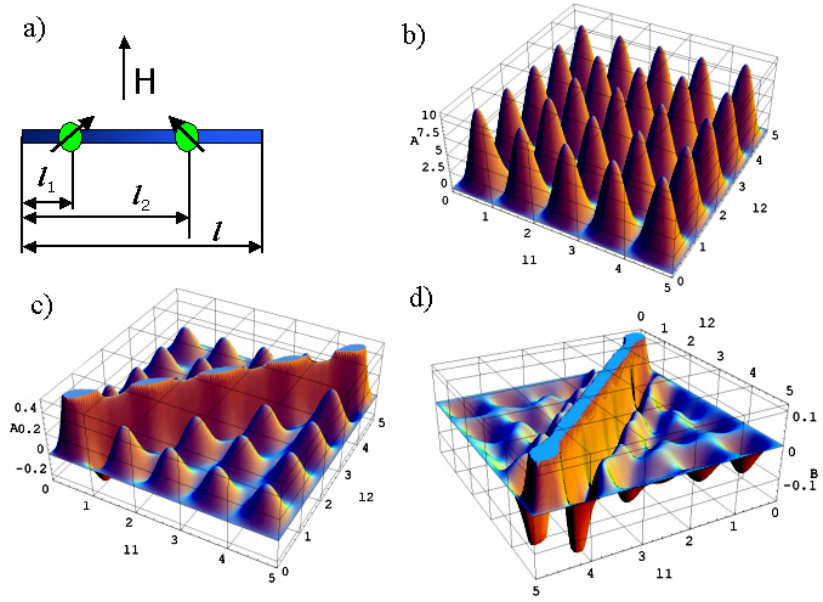

Figure 2. (a) Two nuclear spins embedded in a finite-length quantum wire in a magnetic field; (b) the nuclear spin coupling constant A in a low-magnetic-field region ($\frac{4g\mu_B m_e a^2 H}{\hbar^2\pi^2} = 0.1$); (c) the nuclear spin coupling constant A in a high-magnetic-field region ($\frac{4g\mu_B m_e a^2 H}{\hbar^2\pi^2} = 3$); and (d) the 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 $E_w = \frac{\hbar^2\pi^2}{2m^* l^2 a}$.)

In what follows we will consider the system in the envelope function approximation; the rapidly varying function $u_0'(\boldsymbol{r})$ appears only in the expression for the hyperfine interaction. The Hamiltonian of the system is given by $H = H_0 + H_1^{(1)} + H_1^{(2)}$ with

$$H_0 = \frac{1}{2m^*}\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 + V(\boldsymbol{r}) - g\mu_B\boldsymbol{\sigma}\cdot\boldsymbol{H} \tag{3}$$

and

$$H_1^{(i)} = \frac{8\pi}{3}\mu_B\hbar\gamma_n|u_0'(\boldsymbol{r}_i)|^2\boldsymbol{\sigma}\cdot\boldsymbol{I}_i\delta(\boldsymbol{r}-\boldsymbol{r}_i) \tag{4}$$

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, $\boldsymbol{A}$ is the vector potential, g is the electron g-factor, μ_B is the Bohr magneton, $\boldsymbol{H}$ is the magnetic field, γ_n is the nuclear gyromagnetic ratio, $\boldsymbol{I}_i$ and $\boldsymbol{\sigma}$ are nuclear and electron spins, $\boldsymbol{r}_i$ is the radius vector of nucleus i ($i = 1, 2$). Because the electron wavefunction is strongly peaked on the nuclei, the contact hyperfine interaction energy greatly exceeds the dipolar spin interactions.

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

$$E = \sum_{E_i, E_f} \frac{\langle\Psi_i|H_1^{(1)}|\Psi_f\rangle\langle\Psi_f|H_1^{(2)}|\Psi_i\rangle}{E_f - E_i} f_i(1-f_f) + \text{c.c.} \tag{5}$$

Here Ψ_i and E_i are eigenfunctions and eigenvalues of H_0 and f_i is the electron distribution function. In this paper 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. The 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.

2.1. 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 $\boldsymbol{H}$ in the z-direction, with two nuclear spins located at $\boldsymbol{r}(\rho, \varphi, z) = \boldsymbol{r}_1(a + d/2, \varphi_1, h/2)$ and $\boldsymbol{r} = \boldsymbol{r}_2(a + d/2, \varphi_2, h/2)$ (figure 1(a)). In this subsection we use polar coordinates. The electron confining potential $V(\rho, z)$ is

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

First, let us find eigenfunctions and eigenvalues of the Schrödinger equation with the Hamiltonian (3). Due to the axial symmetry of the ring, the wavefunction can be written as follows:

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

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

$$-\frac{\hbar^2}{2m^*} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} R_{m,n} + \frac{\hbar^2}{2m_e \rho^2} \left(m + \frac{\Phi(\rho)}{\Phi_0} \right)^2 R_{m,n} = E_{m,n} R_{m,n}, \tag{8}$$

where Φ_0 is the magnetic flux quantum and the radial number $n = 1, 2, 3, \ldots$. The boundary conditions imposed by the potential $V(\rho, z)$ (6) are: $R_{m,n}(a) = 0$ and $R_{m,n}(a + d) = 0$.

We will look for the solution of equation (8) assuming that at $d \ll a$ the vector potential varies slowly in the ring, so we can put $\Phi(\rho) \simeq \Phi(a + d/2)$. In this case the solution of equation (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 $A = |m + \frac{\Phi(a+d/2)}{\Phi_0}|$ and $\alpha_{m,n} = \sqrt{\frac{2m_e E_{m,n}}{\hbar^2}}$, and the constants C_1, C_2 and energy levels $E_{m,n}$ are defined by boundary conditions and the normalization condition $\int_a^{a+d} \rho R^*_{m,n}(\rho) R_{m,n}(\rho)\, \mathrm{d}\rho = 1$. Unfortunately, a wavefunction of the form (9) allows only numerical calculation of the effective nuclear spin interaction.

To obtain an analytical result, consider the effective interaction energy constants A and B for the case of an 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 the wavefunction decouples from the orbital part, $R_n(\rho) = \sqrt{\frac{2}{d}} \sin(\frac{(r-a)\pi n}{d})$ and

$$E_{n,m,s=\pm} = \frac{\hbar^2}{2m^*} \left(\frac{\pi n}{d} \right)^2 + \frac{\hbar^2}{2m^* a^2} \left(m + \frac{\Phi(a + d/2)}{\Phi_0} \right)^2 \mp g \mu_B H/2. \tag{10}$$

For the infinitely narrow ring it is reasonable to consider only the states with $n = 1$. With equation (5), 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 $K_r = 2(\frac{16}{3adh}\Omega\mu_B\hbar\gamma_n|u_0'(0)|^2)^2$.

Using the wavefunction in the form of equation (7), we numerically calculate the magnetic field dependences of the nuclear spin interaction constants A and B using the following set of parameters: $\varphi_1 = 0$, $\varphi_2 = \pi$, $a = 100$ nm, $h = 1$, $d = 1$ and 0.5 nm, one electron in the ring, $T = 0$. The results of our calculations are shown in figure 1(b). The magnetic field dependences of the effective nuclear spin interaction constants are governed 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, which gives a $1/H$ dependence of the interaction amplitude. The nuclear spin coupling constant B is connected to 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 where there are two ground states, function B has discontinuities. In this case the perturbation theory is not applicable. The result obtained is in good agreement with the result obtained for the case of infinitely narrow-ring potential equations (11), (12).

2.2. Nuclear spin interaction in mesoscopic wires

The next system under consideration is a finite-length quantum wire of the length l in the x-direction, of thickness d and of height h, with two nuclear spins located at $\boldsymbol{r}(x, y, z) = \boldsymbol{r}_1(l_1, d/2, h/2)$ and $\boldsymbol{r} = \boldsymbol{r}_2(l_2, d/2, h/2)$ in a magnetic field $\boldsymbol{H}$ in the z-direction (figure 2(a)). We suppose that the transverse sizes of the quantum wire are much smaller than the length of the quantum wire and the cyclotron orbit of the electron. We consider a model where the confining potential is

$$V(x) = \begin{cases} 0 & \text{if} \quad 0 \leqslant x \leqslant l, 0 \leqslant y \leqslant d, 0 \leqslant z \leqslant h \\ \infty & \text{otherwise.} \end{cases} \tag{13}$$

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

$$\Psi_{n,m,k,\pm} = \sqrt{\frac{8}{ldh}}\left(\begin{pmatrix}1\\0\end{pmatrix}, \begin{pmatrix}0\\1\end{pmatrix}\right) \sin\left(\frac{n\pi x}{l}\right) \sin\left(\frac{m\pi y}{d}\right) \sin\left(\frac{k\pi z}{h}\right), \tag{14}$$

$$E_{n,m,k,\pm} = \frac{\hbar^2\pi^2}{2m^*l^2}n^2 + \frac{\hbar^2\pi^2}{2m^*d^2}m^2 + \frac{\hbar^2\pi^2}{2m^*h^2}k^2 \mp g\mu_B H/2, \tag{15}$$

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 equations (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 functions of nuclear spin positions for odd and even numbers of electrons N in the wire. The results of the calculation for the odd number of electrons $N = 9$ at $T = 0$ are presented in

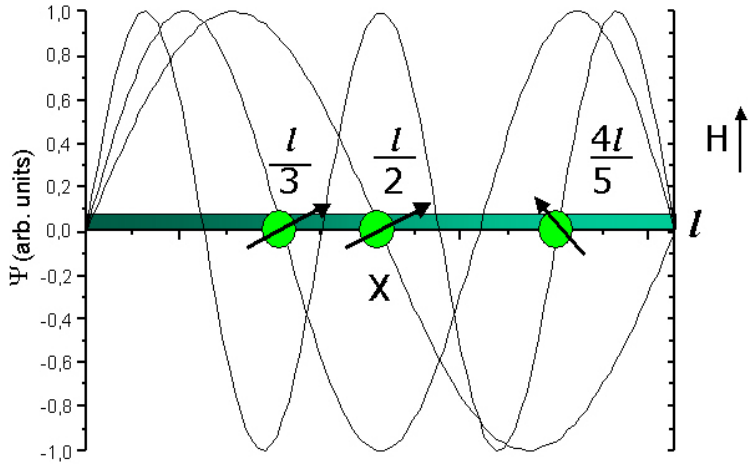

Figure 3. The qubit arrangement and the last occupied electron level wavefunction for $N = 3, 5, 9$ electrons in the wire. The qubits are located in the nodes of the different wavefunctions.

figures 2(b)–(d). In the low-magnetic-field region, when the Zeeman splitting energy is much less than the energy gap between levels with different n (equation (15)), and at the $T = 0$ limit, the expression for A takes a simple form:

$$A = K\frac{\left(\sin\left(\frac{(N+1)\pi l_1}{2l}\right)\sin\left(\frac{(N+1)\pi l_2}{2l}\right)\right)^2}{g\mu_B H}. \tag{16}$$

where $K_w = 2\left(\frac{64\pi\Omega\mu_B\hbar\gamma_n|u_0'(0)|^2}{3ldh}\right)^2$. In this limit the interaction constant A has a set of $\frac{(N+1)^2}{4}$ maxima (figure 2(b)) and $B \ll A$. Figure 2(c) shows an increasing of the 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 the interaction constant A for the other nuclear spin positions with increasing magnetic field. The interaction constant B has a non-trivial dependence on the nuclear spin positions (figure 2(d)).

3. Conclusions and discussion

To conclude, we proposed a new possible implementation of a basic unit for quantum computers based on the nuclear spin qubits embedded in 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 the indirect nuclear spin interaction in 2D and 3D metals. Preliminary finite-temperature calculation indicates that the values of the effective nuclear spin interaction constants decrease with temperature, but the main features of the results obtained remain qualitatively unchanged.

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

(1) It is well known that nuclear spins are appropriate candidates for being qubits [6, 10]. Nuclei with spin 1/2 are two-level systems with well defined states $|0\rangle$ and $|1\rangle$. Needless

to say, such a system is scalable and, basically, there is no limitation in principle on the reasonable number of nuclear spin qubits which can be integrated into a quantum circuit. The ring architecture of the quantum computer has considerable promise. Let us imagine a mesoscopic ring with nuclear spin qubits located in its immediate vicinity. A local change of the electrostatic potential near a qubit caused by a gate electrode changes the value of the envelope wavefunction on the qubit and, correspondingly, allows one to switch on the interaction between any two qubits, whereas in almost all quantum computer proposals 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 general agreement that this is the only feasible method, since the nuclear spins are highly isolated from the environment. The possibility of nuclear spin polarization by spin-polarized transport was demonstrated almost ten years ago [24, 25]. Possible methods for introducing non-equilibrium 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 for performing the quantum computation, since the discrete electron spectrum in mesoscopic systems imposes restrictions on the flip–flop processes, and the nuclear spin relaxation time at low temperatures is expected to have an activation behaviour [13]. Up to the present, a calculation of the nuclear spin decoherence time in mesoscopic structures has not been made; however, as a rough estimation we can take the decoherence time of the nuclear spin qubit embedded in a 2DEG, $T_2 = 10$ s [10]. The characteristic time of qubit interaction is $T_{int} \sim h/A$, where for the nuclear spin qubits in a finite-length quantum wire, A is given by equation (16). Using available experimental data for GaAs, $|u_0'(0)|^2_{^{75}\mathrm{As}} = 9.8 \times 10^{25}$ cm^{-3} [19], and the following set of parameters: $a = 200$ nm, $d = h = 5$ nm, $H = 0.01$ T, we obtain $T_{int} = 2 \times 10^{-5}$ s and $T_2/T_{int} = 5 \times 10^5$. Our estimate indicates that the present system is suitable for use in fault-tolerant quantum computation.

(4) (a) The one-qubit operations using 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 the electron wavefunction on some qubits and zero on the others. 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 β_i are different prime numbers and α_i are integers ($\alpha_i < \beta_i$). The orbital part of the last electron level wavefunction (from equation (14)) for

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

electrons in the system is

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

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 wavefunction and only qubits j and k interact. Figure 3

illustrates this idea. It follows that the accuracy of nuclear spin positioning should be a few atomic units.

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

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