A scalable quantum gate design for quantum computation

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We present a scalable design for a quantum gate based on an electrostatically defined InP/InGaAs quantum dot system. The spin doublet state of an electron trapped under each quantum gate constitutes the desired qubit. A numerical investigation is conducted based on the self-consistent solution of coupled Poisson and Schrödinger equations in the few electron regime. The Gibbs distribution is considered to take into account the discrete charge statistics and the Coulomb blockade effect. The results of the calculation show that the proposed design satisfies the necessary requirements for a quantum gate.

Since the discovery of an exponential speed up in factorization by quantum computing in comparison to the best classical algorithms, interest in the field of quantum information science generally, and in schemes for developing a quantum computer, has increased dramatically [1, 2]. Initial success was forthcoming for developing quantum computers (QCs), especially in terms of interesting proposals, including most notably ion trap systems [3], quantum electromagnetic cavity [4], superconductor Josephson junctions [5], nuclear magnetic resonance [6], nuclear spins in solids [7], and electron spins [8, 9]. A potential system must satisfy the following well-known conditions for quantum computations (see for example Ref. 10): (a) a two-level system defined as a qubit, (b) the possibility to prepare the initial states and to measure each qubit, (c) a controllable source of entanglement to produce the fundamental controlled-not gate operation, and (d) long coherence time. The use of artificially structured solid-state systems to create an ordered array of electron spins offers one of the best possibilities of achieving sufficient coherence time and a pure initial state for useful operation. State-of-the-art nanoscale fabrication and epitaxial growth capabilities are already able to realize the artificial structures consisting of an array of quantum dots (QDs) at the required dimensions. With each QD trapping a single electron at the interface of a heteroepitaxial structure, an array of spins with nearest neighbor coupling is produced. These qubits are addressable with established microwave electron spin resonance or newly emerging g-tensor engineering techniques. Moreover, electron spin relaxation time in the relevant semiconductors can reach the values up to several microseconds [11], providing a sufficiently long coherence time for error correction.

In this paper, we design a quantum gate based on an InP/InGaAs vertical quantum dot (QD) structure and investigate it in the few-electron regime for possible quantum computing applications. A three-dimensional device model is developed based on the self-consistent solutions of the coupled Schrödinger-Poisson equations. Our results show that the proposed structure may be considered as a realistic candidate for spin-based QC with a sufficiently robust bias margin.

The basic design described above relies on trapping a single isolated electron within each QD of an array of nearest neighbor vertical QDs in a heteroepitaxial crystal. Figure 1 shows the schematic drawing of one such element (i.e., quantum gate), which consists of alternating InP and InGaAs layers. The first InGaAs quantum well starting from the top of the structure creates a QD region (i.e., qubit), and the second InGaAs layer is used as a read-out channel [12]. Electron confinement along the growth direction is produced by the band-gap discontinuity of the heterostructure, whereas the constriction in the quantum well plane can be achieved by applying an appropriate voltage to the gate. Similar vertical QDs based on the Si/SiO_2 [13] or SiGe structures (with split gates) [14] showed promising results. The choice of InGaAs-based materials and geometries enables ready integration with a quantum receiver/transmitter system [12, 15].

To analyze this structure, our numerical model solves the coupled Poisson and Schrödinger equations self-consistently. The three-dimensional electrostatic potential $V(\vec{r})$ is obtained from the non-linear Poisson equation:

$$\nabla^2 V(\vec{r}) = -\frac{4\pi e}{\varepsilon}\left[n(\vec{r}) + N_D^+(\vec{r})\right], \qquad (1)$$

where e is the absolute value of the electron charge, ε is the static dielectric constant, $n(\vec{r})$ is the electron concentration, and the $N_D^+(\vec{r})$ is the concentration of ionized impurities. This equation is solved subject to the boundary conditions on the electrostatic potential $V(\vec{r})$. The metallic gate and the ungated surface at the top of the structure are modeled by the Dirichlet boundary conditions taking into account pinning of the chemical potential (0.3 eV for InP). The substrate is assumed to be grounded. Following the approach as in Ref. [16], we divide our structure into the "bulk" and "quantum" regions. In the "bulk" region away from the qubit layer, electrons are treated semiclassically; namely, the Thomas-Fermi approximation is used in order to obtain

the electron concentration:

$$n(\vec{r}) = \begin{cases} \frac{1}{3\pi^2}\left[\frac{2m_e^*}{\hbar^2}(\mu - U(\vec{r}))\right]^{3/2}, & \text{if } U(\vec{r}) < \mu \\ 0, & \text{otherwise.} \end{cases} \quad (2)$$

Here μ is the chemical potential and $U(\vec{r})$ is the effective electron potential. The chemical potential μ can be determined by the charge neutrality condition:

$$\int [n(\vec{r}) - N_D^+(\vec{r})] d\vec{r} = 0\,, \quad (3)$$

where the integration is carried out over the entire bulk region. In this region, the electron potential $U(\vec{r})$ consists of Hartree potential $U_H = -eV(\vec{r})$, where $V(\vec{r})$ is defined by Eq. (1), and the conduction band offset ΔE_c:

$$U(\vec{r}) = -eV(\vec{r}) + \Delta E_c\,. \quad (4)$$

In order to determine the electron concentration $n(\vec{r})$ in the "quantum" region, we need to solve the Kohn-Sham equation:

$$\Big[-\frac{\hbar^2}{2m_e^*}\nabla^2 + U(\vec{r})\Big]\psi_i(\vec{r}) = E_i\psi_i(\vec{r}) \quad (5)$$

with an appropriate electron potential $U(\vec{r})$. The electron-electron interaction in the quantum region is treated using a density functional theory in the local density approximation. The validity of this approximation, even for the systems of one or two electrons, was demonstrated by Ref. 17. Thus, for the electron potential $U(\vec{r})$ in the quantum region, we have

$$U(\vec{r}) = U_H + \Delta E_c + U_{xc}\,, \quad (6)$$

where U_{xc} is the exchange-correlation potential in the form as in Ref. 17. From Eq. (5), we can obtain the electron concentration in the quantum region through the relation:

$$n(\vec{r}) = \sum_i n_i |\psi_i(\vec{r})|^2\,. \quad (7)$$

Here n_i is electron occupancy in each level which is generally a function of the electron energy and the temperature.

To complete the specification of the electron charge density, it is necessary to compute the electron occupation numbers n_i. One might expect that n_i would be given by the Fermi-Dirac distribution and indeed this would be the case if the electrons in the quantum region were delocalized and in contact with the electrodes. In this case, the qubits could exchange electrons with their environment and the total number of electrons in the dot $N = \sum_i n_i$ could take on non-integer values, which is clearly not tolerable in a QC. Hence, one must carefully arrange things so the wavefunctions exhibit a high degree of localization. Then, only an integer number of electrons can occupy the quantum region and this constraint gives rise to what is known as the Gibbs distribution. The number of electrons is determined by minimizing the Gibbs free energy with respect to the integer number of electrons N. The Gibbs free energy is $F(N) = -kT\ \ln[Z(N)]$, where the grand canonical partition function $Z(N)$ is given by [16]

$$Z(N) = \sum_{n_i} \frac{\sum_i n_i E_i - E_H(N) - \mu N}{k_B T}\,. \quad (8)$$

The summation in $Z(N)$ is carried out over all electron configurations $\{n_i\}$ for which $N = \sum_i n_i$. E_H is the Hartree energy for the system of N electrons which can be calculated in the usual way by using Eq. (7).

In the actual design, we require primarily that the quantum gate trap and maintain one electron in the QD layer with a sufficiently large window of operation. In addition, the energy separation between the QD ground and first excited states should be as large as possible (e.g., larger than the thermal and Zeeman energies). As for the read-out channel, the detailed electron occupancy is not crucial so long as its influence on the QD region is not significant. Hence, we only require the presence of electrons. In an integrated device, the read-out channel will be controlled by additional contacts (see, for example, Ref. 12). Due to the large parameter space involved in this study, an analytical model [18] is employed for preliminary screening followed by self-consistent numerical calculations. For simplicity, a cylindrical symmetry is assumed in the in-plane direction.

Table I summarizes the parameters of one design that satisfies the basic requirements. Roughly speaking, the structure has the gate diameter of approx. 60 nm and the InGaAs quantum well widths of approx. 30 nm. The layers are undoped except at the ground contact. We also consider two optional δ-doped regions in the InP barriers (see Fig. 1).

The results of self-consistent numerical simulations are presented in Figs. 2 and 3. The energy of the ground and the first excited states for the doped and undoped cases (i.e., with and without the δ-doping) are plotted in Fig. 2 as a function of the applied gate voltage. In both cases, the energy levels decrease with increasing gate voltage. Due to the lack of screening charges in the top InP layer, this decrease is much more drastic in the undoped case until the electrons start to occupy the QD region. However, a close examination of the energy spectrum reveals that the separation between the ground and first excited energy levels is almost constant in the range of applied voltages (approximately 0.25 meV in the undoped case and 0.2 meV in the doped case). A typical ground state wavefunction in the QD is plotted for the applied voltage of 0.35 V as a function of the real-space coordinates.

The crucial electron occupancy in the QD is presented in Fig. 3. Clearly, the result indicates that both cases can capture and maintain one electron in each QD with a sufficiently large bias margin, thus demonstrating their

feasibility. For the undoped case, the threshold voltage (i.e., the minimum gate bias to charge the QD with the first electron) is close to 0.3 V along with the bias margin of approximately 90 mV. For the doped case, the situation is less desirable. As expected, the threshold voltage is shifted to a lower value of 0.2 V accompanied by a substantially smaller operating window of 50 mV. The design is relatively insensitive to the structural fluctuations.

In summary, we presented a practical quantum gate design for a possible *QC* application based on a system of coupled QDs. Our model shows that the bias margin for single electron trapping can be as large as 90 mV. The relative robustness of the calculation results demonstrates the potential of our design.

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[1] A. Ekert and R. Jozsa, Rev. Mod. Phys. **68**, 733 (1996).
[2] C. H. Bennett and D. P. DiVincenzo, Nature (London) **404**, 247 (2000).
[3] J. I. Cirac and P. Zoller, Phys. Rev. Lett. **74**, 4091 (1995).
[4] Q. A. Turchette, C. J. Hood, W. Lange, H. Mabuchi, and H. J. Kimble, Phys. Rev. Lett. **75**, 4710 (1995).
[5] A. Shnirman, G. Schön, and Z. Hermon, Phys. Rev. Lett. **79**, 2371 (1997).
[6] I. L. Chuang, N. Gershenfeld, and M. Kubinec, Phys. Rev. Lett. **80**, 3408 (1998).
[7] B. E. Kane, Nature (London) **393**, 133 (1998).
[8] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[9] R. Vrijen, E. Yablonovitch, K. L. Wang, H. W. Jiang, A. Balandin, V. Roychowdhury, T. Mor, and D. DiVincenzo, Phys. Rev. A **62**, 012306 (2000).
[10] A. Steane, Rep. Prog. Phys. **61**, 117 (1998).
[11] J. M. Kikkawa and D. D. Awschalom, Phys. Today **52**(6), 33 (1999).
[12] E. Yablonovitch, H. W. Jiang, H. Kosaka, H. D. Robinson, D. S. Rao, and T. Szkopek, Proc. IEEE **91**, 761 (2003).
[13] A. A. Kiselev, K. W. Kim, and W. C. Holton, in *TECHCON2000* (Semiconductor Research Corporation, Research Traingle Park, NC, 2000), p. 116.
[14] M. Friesen, P. Rugheimer, D. E. Savage, M. G. Lagally, D. W. van der Weide, R. Joynt, and M. A. Eriksson, Phys. Rev. B **67**, 121301 (2003).
[15] A. A. Kiselev, K. W. Kim, and E. Yablonovitch, Appl. Phys. Lett. **80**, 2857 (2002).
[16] S. Nagaraja, P. Matagne, V.-Y. Thean, J.-P. Leburton, Y.-H. Kim, and R. M. Martin, Phys. Rev. B **56**, 15752 (1997).
[17] J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[18] This model uses a single particle Schrödinger equation for the electronic wave function and a Poisson equation for the electrostatic potential. Analytic expressions for the electron energy levels in the QD are then obtained using a combination of harmonic and square well approximations to the electrostatic potential. For more details, see: R. E. Caflisch and L. Y. Cheng, UCLA CAM Report 01-30, November 2001.

Table I: Composition and doping profiles of the proposed quantum gate structure. The InGaAs layers are lattice matched to InP (i.e., $In_{0.53}Ga_{0.47}As$).

Parameter	Value
Top InP thickness ($\AA$)	1108
Top InGaAs thickness ($\AA$)	290
Middle InP thickness ($\AA$)	878
Bottom InGaAs thickness ($\AA$)	355
Bottom InP thickness ($\AA$)	2000
Gate radius ($\AA$)	310
Top InP δ-doping density (cm^{-3})	2.5×10^{19}
Top δ-InGaAs separation ($\AA$)	692
Bottom InP δ-doping density (cm^{-3})	9.7×10^{18}
Bottom δ-InGaAs separation ($\AA$)	550
Width of δ-doped regions ($\AA$)	15

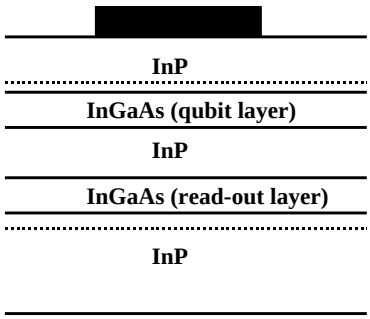

FIG. 1: Schematic representation of the proposed quantum gate structure. The dashed lines denote the δ-doping regions.

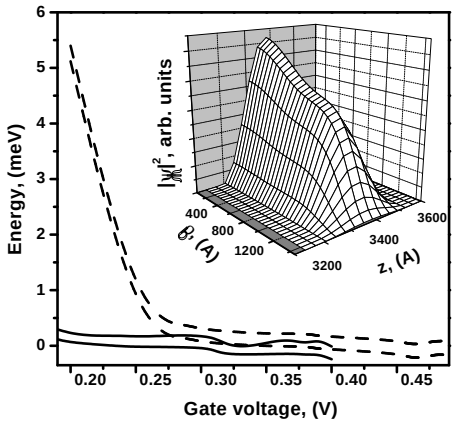

FIG. 2: Energy levels of the ground and first excited states versus applied voltage for the undoped (dash line) and doped (solid line) cases. The inset shows the ground state wavefunction for the undoped structure at 0.35 V. The reference point $z = 0$ in the z direction is set to the bottom of the structure.

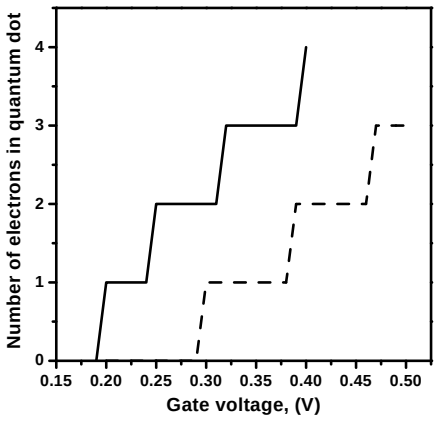

FIG. 3: Electron occupancy in the QD versus applied voltage for the undoped (dash line) and doped (solid line) cases.