Towards a feasible implementation of quantum neural networks using quantum dots

M. V. Altaisky and N. N. Zolnikova
Space Research Institute RAS, Profsoyuznaya 84/32, Moscow, 117997, Russia

N. E. Kaputkina
National Technological University "MISIS", Leninsky prospect 4, Moscow, 119049, Russia

V. A. Krylov
Joint Institute for Nuclear Research, Joliot Curie 6, Dubna, 141980, Russia

Yu. E. Lozovik
Institute of Spectroscopy, Troitsk, Moscow, 142190, Russia

Nikesh S. Dattani
Quantum Chemistry Laboratory, Kyoto University, Kyoto, 606-8502, Japan and
School of Materials Science and Engineering, Nanyang Technological University, 639798, Singapore

(Dated: Mar 17, 2015)

We propose an implementation of quantum neural networks using an array of single-electron quantum dots with dipole-dipole interactions. We demonstrate that this implementation is both feasible and versatile by studying it within the framework of GaAs based quantum dot qubits coupled to a reservoir of acoustic phonons; a system whose decoherence properties have been experimentally and theoretically characterized with meticulous detail, and is considered one of the most accurately understood open quantum systems. Using numerically exact Feynman integral calculations, we have found that the quantum coherence in our neural networks survive for several ns even at liquid nitrogen temperatures (77 K), which is three orders of magnitude higher than current implementations which are based on SQUIDs operating at temperatures in the mK range. Furthermore, the previous quantum dot based proposals required control via manipulating the phonon bath, which is extremely difficult in real experiments. An advantage of our implementation is that it can be easily controlled, since dipole-dipole interaction strengths can be changed via the spacing between the dots and applying external fields.

PACS numbers: 03.67.Lx, 73.21.La, 72.25.Rb

Quantum neural networks (QNNs) have earned tremendous attention recently since Google and NASA’s Quantum Artificial Intelligence Lab announced their use of D-Wave processors for machine supervised learning and big data classification [1, 2]. However, these machines use SQUIDs, which require temperatures in the mK range in order to keep quantum coherence for sufficiently long [3]. This limitation would be lifted by orders of magnitude when the neural network is implemented with quantum dots, which we show have coherence survival times on the ns scale even at 77 K.

Quantum dots (QD) are small conductive regions of semiconductor heterostructure that contain a precisely controlled number of excess electrons, and have been the subject of several excellent reviews, such as [4–6]. The electrons are locked to a small region by external electric and magnetic fields which define the shape and size of the dot, typically from a few nanometers to a few hundred nanometers in size. Controllable QDs are often made on the basis of a 2D electron gas of GaAs heterostructures. The energy levels of QDs are precisely controlled by the size of the dot and the strength of external electric and magnetic fields [7–13]. By arranging the quantum dots in a regular array on a layer of semiconductor heterostructure one can form a matrix for a quantum register, composed of either charge-based, or spin-based qubits, to be used for quantum computations [14].

The fact that QDs can easily be controlled [13] makes arrays of quantum dots particularly attractive for quantum neural networks, where the coherence requirements are not as strict as in circuit-based quantum computing; instead the system just needs to find the minimum of an energy functional, which can be found quicker with the assistance of quantum tunneling rather than solely classical hopping [3].

Using an array of GaAs QDs for quantum neural networks was first proposed by Behrman et al. [16]. Their original idea assumed the use of quantum dot molecules interacting with each other only by means of their shared phonon bath. Within this framework, it would be nearly impossible to control the training of the QNN since manipulating a phonon bath is an arduous task [17]. In this Letter we present a more achievable quantum dot based QNN architecture, where the QDs interact with each other via dipole-dipole coupling. We present realistic physical parameters for all couplings, and use a numerically exact
Feynman integral calculation to study the time evolution of the phonon-damped coherence in a pair of one-electron QDs in such a network.

A careful series of experiments on decoherence rates in SQUIDs was reported in [18], which showed that at 80 mK decoherence rates can be as high as 0.11 ns$^{-1}$, but it is well known that superconducting devices cannot operate at much higher temperatures. We will present numerically exact calculations to show that the quantum coherence in our quantum dot based architecture survives for durations on the same time scale, but at much higher temperatures. All calculations can be regenerated with our open source code and input file provided in the Supplemental Material.

We consider small QDs of $d = 4.5$ nm diameter in a GaAs based substrate [19], where the excitons interact with their bath of acoustic phonons [19–21]. The Hamiltonian of a pair of QD excitons embedded in a semiconductor heterostructure can be written in the form

$$ H = H_{\text{Ex}} + H_{\text{Ph}} + V \equiv H_0 + V, \quad (1) $$

describes the energy of the excitons, with $\Delta_i$ being the energy gap between the ground state and the first excited state of the $i$-th exciton; $K_i$ is a coupling due to an external driving field, $J_{ij}$ is the dipole-dipole coupling between the dots, constructed in analogy to the dipole-dipole interaction of atoms [22]. The pseudo-spin operators of the $i$-th QD are

$$ \sigma^{(i)}_z = |X_i\rangle\langle X_i| - |0_i\rangle\langle 0_i|, \quad \sigma^{(i)}_+ = |0_i\rangle\langle X_i| + |X_i\rangle\langle 0_i|, \quad \sigma^{(i)}_- = |0_i\rangle\langle 0_i|, \quad \sigma^{(i)}_0 = |X_i\rangle\langle X_i|. $$

The free phonon Hamiltonian is

$$ H_{\text{Ph}} = \sum_\alpha \frac{p_\alpha^2}{2m_\alpha} + \frac{m_\alpha \omega^2_a x_\alpha^2}{2}, \quad (3) $$

and the interaction between the phonons and the QDs is given by

$$ V = \sum_{\alpha,i} g_\alpha x_\alpha |X_i\rangle\langle X_i|. \quad (4) $$

We consider a pair of identical QDs ($\Delta_1 = \Delta_2 = \Delta, J_{12} = J_{21} = J, K_1 = K_2 = K$) in which we can see that in the limit of vanishing driving field ($K \to 0$) the eigenstates of $H_{\text{Ex}}$ are

$$ |X0\rangle, |0X\rangle, \frac{|X0\rangle + |0X\rangle}{\sqrt{2}}, |00\rangle, |XX\rangle \quad (5) $$

corresponding to the eigenvalues $(-J, J, -\Delta, \Delta)$. The first two states of Eq. (5) have zero eigenvalue with respect to the interaction with phonons, given by Eq. (4), and thus survive in coherent superposition even in the presence of a bath of acoustic phonons.

We will choose the energy gap $\Delta$ based on the QD diameter $d = 4.5$ nm [19], $\hbar \omega = \frac{2m_1 c^2}{\hbar k r_0} \approx 0.853$ ps$^{-1}$, where $a_0 = \frac{kr_0}{2m_1 c^2} = 3.94$ nm is the Bohr radius of the QD, and $E_0 = \frac{2m_1 c^2}{\hbar k r_0^3} \approx 36.5$ meV [18]. For the dipole frequency we use the estimation [13, 22]: $J = \frac{1}{\hbar} \frac{|e| r_0}{\mu} \approx 0.111$ ps$^{-1}$, where $\varepsilon$ is the dimensionless dielectric constant of GaAs, $L = 100$ nm is a typical inter-dot distance, and $\mu = \langle X0|e|x|00\rangle \approx 108$ Debye is the transition dipole moment of the QDs.

In matrix form the exciton Hamiltonian is then written as

$$ H_{\text{Ex}} = \begin{pmatrix} \Delta & K & K & 0 \\ K & 0 & J & K \\ K & J & 0 & K \\ 0 & K & K & -\Delta \end{pmatrix}, $$

where we assume $K = 0.03$ ps$^{-1}$ is the driving field parameter, which corresponds to low intensity fields of about 88 V/cm.

The system of QDs interacting with phonons can be described in terms of the von Neumann equation for the reduced density matrix

$$ \dot{\rho} = \text{tr}_\text{Ph} \left( -\frac{i}{\hbar} [H, \rho_{\text{tot}}] \right), \quad (6) $$

Eq. (6) can be solved numerically exactly using the quasi-adiabatic propagator path integral (QUAPI) technique [23] using the free open source MATLAB code FeynDyn [24]. We use the initial condition:

$$ \rho_{\text{tot}}(0) = \rho(0) \otimes e^{-\frac{\beta H_{\text{Ph}}}{\hbar}}, \quad \text{where} $$

$$ \rho(0) = |\psi(0)\rangle\langle \psi(0)| , \quad |\psi(0)\rangle = \frac{1}{\sqrt{2}} (|0X\rangle + |X0\rangle), \quad (7) $$

and we treat the phonon bath as continuous, by defining the spectral density:

$$ J(\omega) = \frac{x_0}{m_\alpha \omega_\alpha} \delta(\omega - \omega_\alpha). \quad (8) $$

The spectral density $J(\omega)$ for acoustic phonons in GaAs QDs is extremely well characterized. The form for $J(\omega)$ has been derived from first principles, and the agreement with experiments is within the error bars of the experiment [17]:
with $\alpha = 0.027\pi ps^2$ and $\omega_c = 2.2 ps^{-1}$. This form for $J(\omega)$ along with these specific parameters have been used consistently in a plethora of studies, in the excellent agreement between experiment and theory [1, 21, 24, 26].

In the Feynman integral representation of Eq. 6 the spectral density and temperature determine the bath correlation function [26]:

$$R(t) = \int_0^\infty \frac{d\omega}{\pi} J(\omega) \left[ \cos(\omega t) \coth \left( \frac{\omega}{2k_B T} \right) - i \sin(\omega t) \right],$$

which in turn determines the time scale of the QD’s memory. For the specific spectral density form and parameters used here, it has been shown that the memory lasts for about 2.5 ps [22]. Therefore, having now defined all physical parameters used in the Hamiltonian, we determined through numerical experiments that a time step of $\Delta t = 1$ ps was sufficient for numerical convergence of the Feynman integral, and to ensure that the full memory length of 2.5 ps was captured, we set the memory length in the Feynman integral to 3 time steps.

Converged Feynman integral calculations for all elements of the QD density matrix $\rho(t)$ were obtained at temperatures of $T = 77$ K and 300 K, and in Fig. 1 it is shown that the coherence $\langle X0 | \rho(t) | XX \rangle$ lasts for several ns even at $T = 77$ K.

The decoherence rate $\gamma$ of an off-diagonal density matrix element with respect to time, can be defined by fitting the damped oscillations of that element to a decaying exponential: $e^{-\gamma t}$. To study the dependence of the decoherence rate with respect to temperature, we calculated the dynamics at 30 different temperatures between 5 K and 300 K, and for each case we fitted $\Re[\langle X0 | \rho(t) | XX \rangle]$ to a decaying exponential to determine a decoherence rate $\gamma$.

In a detailed experimental study on SQUIDs [18], it was shown that decoherence rates can be as high as $0.11$ ns$^{-1}$ at 80 mK. Furthermore, superconducting devices are restricted because they do not work above a critical temperature $T_c$. In our Fig. 2 we show that the decoherence rate of $0.11$ ns$^{-1}$ is maintained, even at 8 K, which is three orders of magnitude greater in temperature to the SQUID study of [18]. Furthermore, decoherence rates better than $1$ ns$^{-1}$ are still maintained even at $77$ K which is accessible by liquid nitrogen.

**FIG. 2.** The decoherence rate remains on the 1 ns$^{-1}$ scale at temperatures accessible by liquid nitrogen (77 K).

**Discussion.** The idea of a quantum neural network [27] is to connect a set of quantum elements, in our case the QD excitons, by tunable weights $J_{ij}$, so that a certain quadratic optimization problem given by the weight matrix becomes a physical problem of evolving a quantum system at non-zero temperature towards the minimum energy state. The dissipative bath in fact plays an integral role in this quantum annealing process [28, 29]. This is different from a QNN implemented as a circuit-based quantum computer [30], where the interaction with the environment poses the main obstacle for creation of stable superpositions of quantum states. In a quantum annealer the interaction of the system with the environment, i.e., the noise, in contrast can increase the effective barrier transparency between the local minima and the desired ground state, therefore enhancing the efficiency of the computation [31, 32].

Present solid state quantum annealing computers [3, 33] are based on SQUID qubits with programmable weights implemented as inductive couplings between the SQUIDs. Such systems operate at the temperatures much below 1K, requiring power on the kW range for cooling the system. In an array of dipole-dipole coupled QDs with a low driving frequency the coupling weights $J_{ij}$ can be tuned by either external fields and/or by changing material properties in the area between the dots, and we have shown using a numerically exact approach that such devices can maintain coherence at 77 K.

The difference between our design described by the
Hamiltonian \([2]\) and the classical Hopfield neural network with the \(J_{ij}s_i^z s_j^z\) interactions, as well as quantum annealers on SQUIDs, is that the interaction \(J_{ij}\sigma_i^+ \sigma_j^-\) flips the states of two interacting qubits dynamically, in the presence of a fluctuating environment. In this sense our model is closer to the biological settings of the original Hopfield work \([34]\) than the spin glass type energy minimizing models. The Hamiltonians considered in this Letter can be used both for networks with self-organization and feed-forward networks \([35]\).

The possible application of QDs to the construction of quantum neural networks has already been discussed in the literature \([16, 36]\). These considerations however involve only the problem of charge control of the qubit state and requires manipulation of the phonon bath in order to work. In the present Letter, we have introduced an element of a quantum dot neural network architecture which is easily tuned via the spacings between the dots and external fields, including local charge deposition and plasmons affecting locally the space between dots \([37]\). We strongly advocate for dipole-dipole coupled QDs as an architecture for the construction of quantum neural networks that are robust and feasible at higher temperatures than current SQUID-based architectures.

Acknowledgements. The authors have benefited from comments and references given by E. C. Behrman and R. G. Nazmitdinov. The work was supported in part by RFBR projects 13-07-00409, 14-02-00739 and by the Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of MISiS. NSD thanks the Oxford University Press for financial support through the Clarendon Fund, and acknowledges further support from NSERC/CRSNG of/du Canada, JSPS for a short-term fellowship in Japan, and the Singapore NRF through the CRP under Project No. NRF-CRP5-2009-04.