Effect of image charge on double quantum dot evolution

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\begin{abstract}
A charge-based qubit is subject to image forces originating in nearby metal gates. Displacement of charge in an oscillating qubit indispensably results in moving charges in metal. Therefore, Joule loss is one more source of qubit decoherence. We have estimated the quality of Rabi oscillations for a realistic double-quantum-dot as $Q \sim 100$. This kind of decoherence cannot be suppressed by lowering temperature as it is evoked by surface roughness scattering of electrons which is almost insensitive to temperature. Possibilities to avoid such a decoherence are briefly discussed. The effect of energy dissipation and image charge potential on qubit dynamics is studied by means of a specific local-in-time non-Markovian master equation.
\end{abstract}

1. Introduction

Charge-based qubits look quite promising for a solid state quantum computer implementation. However, almost all proposals of such qubits include the gates for their operation. At the same moment, it is well known that gates can cause decoherence\textsuperscript{1} in the system, in particular, via the thermal noise in a gate voltage \cite{1}, carrier injection \cite{2} or phonons \cite{3–5}. A good point is that in the system, in particular, via the thermal noise in a gate voltage \cite{1}, carrier injection \cite{2} or phonons \cite{3–5}. A good point is that the moving charge in the qubit creates a moving charge in the gate which indispensably entails a resistivity loss. A direct observation of decoherence due to image charges was presented in the interference experiment with electrons flying over the metal surface \cite{6}. A similar effect with regard to qubits was firstly emphasized in Ref. \cite{7} and then developed in Ref. \cite{8}. The preceding papers \cite{9,10} discussing a resistivity loss of a charged particle moving along a metal surface did not take into account a screening and thus underestimated the loss by many orders of magnitude compared to that in Refs. \cite{7,8}.

Although the ‘image charge’ is virtually located deep inside the metal, it is produced by surface charge distribution, which is extremely sensitive to the surface roughness. This entails a dramatic increase of decoherence rate and we point out this fact in the paper. We have estimated the rate of this loss and recovered that the associated decoherence of the qubit might be substantial in actual devices. Certainly, the feasible way to avoid it lies in employment of superconducting materials for gate electrodes. Nevertheless, it should be pointed out that many proposals of quantum computers exploit strong magnetic fields (e.g., Ref. \cite{1}) and thin-film metal gates with rough surface scattering. Both circumstances may entail a dissipative current mechanism rather than a superconducting one even at low temperatures (tens of mK). Another possibility to avoid dissipation is to do without gates at all and exploit laser pulses for driving the qubits \cite{11–13}. One more way out lies in employment of qubits based on space states without charge transfer \cite{14,15}.

A presence of a nearby metal surface also causes the qubit dynamics to be rather difficult. It takes place due to a specific nonlinear term in the Schrödinger equation corresponding to a strong attraction to the metal. In the paper, we discuss physical aspects leading to such a peculiar image-force potential. In view of decoherence, one cannot exploit the Schrödinger equation anymore. We derive and solve a specific local-in-time non-Markovian master equation, which takes into account both the decoherence and the image-force potential.

2. Charge qubit and image charge

The structure under consideration is sketched in Fig. 1. It consists of a double quantum dot (DQD) placed near a metal surface which indispensably exists in any structures operated by gates. The DQD contains one electron. If an electron were a classical particle, we would deal with a well known problem of...
electrostatics. The solution of this problem is based on introduction of image charge. This charge is of opposite sign and is located symmetrically with regard to the metal surface. As far as quantum electron is concerned, one should resort to the quantum mechanics formalism. But it is not clear whether the image charge approach remains correct. At the first sight the problem is not difficult at all. One should simply add the image-force potential $-e^2/2\varkappa r$ to the confining potential of the DQD, where $e$ is an elementary charge, $\varkappa$ is a dielectric permittivity, $r$ is a distance from the electron to the metal surface. The question arises what is the real charge distribution in the metal corresponding to the image charge. Thus the obstacle appears how to introduce an image-force potential into the Schrödinger equation.

The first proposals to solve this problem were made in Refs. [16,17]. Authors suggested that the surface charge distributes itself in response to the instantaneous distribution of an external charge given by $-e^2/2\varkappa r$, where $r=(x, y, z)$, with $z$ being equal to 0 on metal surface. This results in the image-force potential of the form

$$V_{im}(x,y,z,t) = \int_{-\infty}^{+\infty} dx' \int_{-\infty}^{+\infty} dy' \frac{-e^2|\psi(x,y,z',t)|^2 dz'}{\varkappa \sqrt{(x-x')^2 + (y-y')^2 + (z-z')^2}}.$$  

(1)

In Ref. [18] such an image-force potential has been used successfully to calculate a perturbation of atomic energy levels caused by a nearby metal surface. It can be shown that such a potential is a consequence of the Hartree mean-field approach applied to the system ‘metal-qubit’. In fact, it is demonstrated in Ref. [19] that if two interacting subsystems oscillate with far different frequencies, then the Hartree mean-field approach becomes valid. In this particular case such an approach is acceptable because the characteristic time of the electron oscillation in a qubit (period of Rabi oscillations) is much longer than the relaxation time in metals which is of the order of $10^{-13}$ s. These arguments authorize an introduction of the image-force potential (1) and set limits to its applicability. It is worth noting that previously the mean-field approximation was widely used for simulation of quantum many-particle systems interacting with metal gates (see, e.g., Ref. [20]). An electric potential was acquired via a self-consistent solution of the Schrödinger and Poisson equations.

Although the image charge is situated deep under the metal surface, really, it is produced by a distributed charge quite close to the surface (Fig. 1). The thickness of this layer is about the Tomas–Fermi screening length $r_{TF}$, which equals several Ångströms in metals. It is shown in Ref. [21] that if an electron moves along the metal surface with a velocity $v$, then the screening length remains $r_{TF}$ whenever $v \ll v_F$, where $v_F \sim 10^6$ cm/s is the Fermi velocity of metal electrons. For realistic DQDs of a size $d \sim 10$ nm and Rabi frequencies $\nu < 1 $ THz, the characteristic velocity of an electron $\nu \sim d \nu$ surely satisfies the requirement $\nu \ll v_F$. Therefore, the resistivity of screening electrons is determined by a surface roughness scattering rather than a bulk phonon scattering. It is known that, unlike the phonon scattering, the surface scattering is almost independent of temperature.

3. Energy dissipation

Below we present analytical and numerical calculations of the decoherence rate for two models: the first one neglects the size of quantum dots and assumes a classical-like motion of the electron inside a box with the length $d$; the second one takes into account a finite size of quantum dots as well as a quantum behaviour of the electron.

3.1. Model 1: flying electron

When the electron is located in one quantum dot, its wave function resembles the delta function, i.e., the electron can be regarded as a point charge. Oscillations of the electron in the DQD can be roughly treated as transitions of such a charge between quantum dots. The charge density $\rho(x,y,t)$ at the metal surface induced by a point charge moving with a velocity $\nu$ along the surface in $x$-direction at a distance $D$ from the surface is supplied by the solution of the relevant electrostatic problem [22]

$$\rho(x,y,t) = \frac{eD}{2\pi((x-vt)^2 + y^2 + D^2)^{3/2}}.$$  

(2)

The associated surface current density $j(x, y, t)$ obeys the continuity equation

$$\partial \rho \frac{\partial}{\varkappa} + \nabla \times j = 0,$$  

(3)

which gives rise to

$$j_x(x,y,t) = \nu \rho(x,y,t) = \frac{veD}{2\pi((x-vt)^2 + y^2 + D^2)^{3/2}}.$$  

(4)

The Joule loss power $W_j$ is

$$W_j = \int_{-\infty}^{+\infty} \sigma_\tau^2 \int j(x,y,t) dx dy,$$  

(6)

where $\sigma_\tau = \sigma_{\tau TF}$ is a sheet specific conductivity providing $\sigma$ is a bulk specific conductivity of metal near its surface. The screening charge is moving inside a layer of the thickness $r_{TF}$ under the metal surface. The result of integrating Eq. (6) is time independent and reads

$$W_j = \frac{\nu^2 e^2}{16\pi \sigma_{\tau TF} D^2}.$$  

(7)

The Joule energy loss averaged over a period $T$ of Rabi oscillations of the qubit is

$$E_j = W_j T = \frac{e^2 d^2}{8\pi \sigma_{\tau TF} D^2},$$  

(8)

where the relation $v = d/T$ was taken into account.

Finally, the associated quality $Q$ of Rabi oscillations is

$$Q \approx \frac{\hbar v}{E_j} = \frac{8\pi \Delta \sigma_{\tau TF} D^2}{e^2 d^2},$$  

(9)

where $\hbar$ is the Plank constant. If the qubit is placed perpendicular to a metal surface, then the energy loss is lower and the quality is about one order greater.
3.2. Model 2: Winking Electron

Let us consider a typical DQD engineered in 2-dimensional electron gas by gates [23–26]. The confining potential of such a DQD can be approached by two parabolic wells \( V_{\text{conf}} \propto (|x| - d/2)^2 + y^2 \delta(z - D) \), and a localized state of the electron in each dot is described by a Gaussian wave function. Suppose the electron occupies the right dot at the moment \( t = 0 \). Then the probability to find the electron in the right and left dot is \( \cos^2(\Omega t/2) \) and \( \sin^2(\Omega t/2) \), respectively, where \( \Omega = 2\pi v \). The electron charge distribution at the moment \( t \) reads

\[
-\left( \psi_1(z, \eta, \zeta, t) \right)^2 = \Re \left( \psi_1(z, \eta, \zeta, t) \right)^2 \sin^2(\Omega t/2) + \Re \left( \psi_2(z, \eta, \zeta, t) \right)^2 \cos^2(\Omega t/2),
\]

where \( \psi_1(z, \eta, \zeta, t) \) corresponds to Eq. (11) and \( \psi_2(z, \eta, \zeta, t) \) corresponds to Eq. (10). The dominating surface scattering is insensitive to \( \eta \) and \( \zeta \) in formula (1). The metal surface is sensitive to the total electron charge density. For this reason, the surface charge distribution is

\[
\rho_{s(x,y,t)} = \rho_{s(x,y)} \sin^2(\Omega t/2) + \rho_{s(x,y)} \cos^2(\Omega t/2),
\]

where \( \rho_{s(x,y)} = \frac{e}{2\pi a^2} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dy \exp \left( -\frac{(z^2 + y^2)\eta^2}{2\sigma^2} - \frac{z^2 + y^2}{2\sigma^2} \right) \delta(z - D),
\]

and

\[
\rho_{s(x,y)} = \frac{eD}{(2\pi)^2} \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dy \exp \left( -\frac{(z^2 + y^2)\eta^2}{2\sigma^2} - \frac{z^2 + y^2}{2\sigma^2} \right)
\]

Solving the continuity Eq. (3), we obtain

\[
J_s(x,y) = \frac{\rho_{s(x,y)}}{2} \sin \Omega t \int_{-\infty}^{\infty} \left[ \rho_{s(x,y)} - \rho_{s(x,y)} \right] d\phi.
\]

Arguing as above in Model 1, we obtain the quality of Rabi oscillations

\[
Q = \frac{16a^2 \alpha h a}{\epsilon^2 (\alpha - D)},
\]

where we introduced the following dimensionless function:

\[
I(a, d) = \frac{1}{(2\sigma a^2)^2} \int_{-\infty}^{\infty} dx d\phi \int_{-\infty}^{d/2} d\phi' \frac{x^2}{2\sigma^2} \sinh \left( \frac{d^2 - d}{2\sigma^2} \right)^2.
\]

In general case of an arbitrary size of dots \( a \), a distance between them, \( d \), and a distance from the qubit to metal, \( D \), the calculation of function \( I(a, d) \) is rather complicated. Nevertheless, analytical solutions can be found under some assumptions. In the limit of infinitesimal quantum dots \( (a - D) \), integration with respect to \( \zeta \) and \( \eta \) reduces to integration of the delta function, and integration with respect to \( x \) can be performed analytically. The result is

\[
I(0, d) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \left( x + d/2 \right)^2 \left( x - d/2 \right)^2,
\]

Moreover, if the distance between quantum dots is essentially smaller than the distance to the metal, i.e., \( d = D \), then

\[
I(0, d) \approx (\pi/2)d^2. \]

Therefore, in case \( a \ll D \) and \( D \ll D \), the quality of Rabi oscillations is

\[
Q \approx \frac{32 \pi a^2 d^2}{\epsilon^2 d^2},
\]

which is nothing else but a solution of Model 1 with a slightly different prefactor.

3.3. Discussion

In order to estimate the quantity (15), one needs to know the value of a metal conductivity \( \sigma \) in the vicinity of the surface. We point out that the Debye charge is placed within the narrow layer with the thickness of the order of \( \gamma \). The crucial point is the roughness of the metal surface. The mean free path of surface electrons \( l \) is limited by several lattice distances, i.e., \( l \sim 10^{-7} \) cm. Assuming the concentration of free carriers \( n = 10^{22} \) cm\(^{-3} \) and the effective mass \( m^* = 10^{-2} \) g, we have

\[
\sigma \approx \frac{e^2 n}{m^* \gamma} \approx 2 \times 10^{15} \text{ S}^{-1},
\]

instead of relatively great values of bulk conductivity used in Ref. [8]. The dominating surface scattering is insensitive to temperature, therefore, the conventional bulk conductivity rule \( \sigma \sim T^{-3} \) is broken down.

Another important fact is that the quality \( Q \) calculated by either Eq. (9) or Eq. (18)) does not depend on the environment permittivity \( \kappa \). It is a direct consequence of the fact that the total free charge on the metal surface equals \( e \), regardless of the environment permittivity, whereas \( \kappa \) effects only on the bound charge density inside the dielectric (e.g., depleted semiconductor) [22]. Since bound charges do not contribute to the current in the metal and, consequently, to Joule losses, the influence of \( \kappa \) on \( Q \) is eliminated.

The quality \( Q \) is calculated numerically for realistic structures and depicted for fixed \( d \) and \( D \) in Figs. 2 and 3, respectively. Asymptotic solutions \( Q_{a < D} \) and \( Q_{a > D} \) are also illustrated and are in a good agreement with numerical values \( Q \) in corresponding ranges of parameters. In Fig. 3, for \( a = 50 \) nm the condition \( a - D \) is met so one can notice a deviation from analytical expression (15). Nevertheless, in physically implementable double quantum dots \( a \ll D \), the dot can be considered as a single one and it is hardly possible to distinguish between

![Fig. 2. Quality of qubit Rabi oscillations vs. distance to a metal surface. Centers of quantum dots are located 100 nm apart. Lines and points correspond to analytical and numerical solutions, respectively.](image-url)
localized 'left' and 'right' states. The condition \(a \lesssim d\) is satisfied for a few points on the right-hand side of Fig. 3.

For \(D=d=50\) nm and \(a=25\) nm, the results of analytical and numerical calculations are nearly coincident, \(Q \approx 100\). This quality gives rise to the error \(\varepsilon=1\%\) per cycle of a quantum computation algorithm, which is not adequate for a correct performance of the quantum computer requiring \(\varepsilon < 0.001 \text{--} 0.01\%\) [27]. The obtained magnitude of \(Q\) points to the peculiarity of 'qubit-gate' decoherence processes. Dealing with gate-engineered charge qubits, it is hardly possible to achieve the relation \(d \ll D\). Consequently, the decoherence caused by image charge can be a main source of the strong relaxation of Rabi oscillations observed in the experiment with double quantum dots [24–26]. This kind of decoherence is also presented in quantum registers based on trapped ions. In Ref. [28], \(^{24}\)Mg\(^{+}\) ions are confined approximately \(D=40\) µm above planar gold electrodes, with the center-of-mass (COM) mode frequency being \(f \approx 2\) MHz. This means, that the zero-point oscillations have an amplitude \(A = \sqrt{\hbar/(4\pi Mf)} \approx 10\) nm (\(M\) is the mass of a single ion). Substituting \(d=2A\) in formula (18), we obtain the quality of COM-oscillations \(Q \approx 3 \times 10^5\). The corresponding decoherence time is \(\tau = Q/f \approx 150\) s. Thus, the interaction with gates sets an upper limit on the decoherence time.

4. Qubit evolution

In this section, we discuss a quantum behaviour of the qubit subjected to decoherence caused by image charges and also reveal the effect of image-force potential on qubit functioning.

A conventional description of the qubit evolution in presence of environment relies on the Kossakowski–Lindblad equation [29] for the density operator \(\rho\). To define the density matrix \(\rho\) we exploit a basis of nondisturbed Hamiltonian eigenstates, i.e., the symmetric (ground) state \(\ket{0}\) and the antisymmetric (excited) state \(\ket{1}\) of the electron inside the double quantum dot. Then such an equation yields

\[
\frac{d\rho}{dt} = -i\frac{\hbar}{2}[H,\rho] + \gamma(2\sigma_\rho\rho - \rho\sigma_\rho - \sigma_\rho\rho)
\]

(20)

where \(\gamma\) is the transition rate from \(\ket{1}\) to \(\ket{0}\); \(\sigma_- = \ket{0}\bra{1}\) and \(\sigma_+ = \ket{1}\bra{0}\); \([A,B] = AB - BA\) and \((A,B) = AB + BA\) are commutator and anticommutator, respectively.

For our particular problem and choice of the basis, the transition rate \(\gamma\) coincides with the energy dissipation rate divided by \(\hbar\). Using results of Section 3, it is not hard to see that

\[
\gamma = \gamma(t) = \frac{1}{\hbar Q}[\frac{d}{dt}(\varrho_{10} + \varrho_{11})^2]
\]

(21)

and, consequently, depends on time. For example, \(\gamma = 0\) if \(\varrho_{10} = (\ket{1}\bra{1})\) or \(\varrho_{10} = (\ket{0}\bra{0})\). Actually, the qubit dynamics (20) with the time-dependent damping coefficient (21) is a specific local-in-time non-Markovian master equation [30], where the decay rate becomes state dependent. From the viewpoint of quantum information theory, the evolution of the qubit is governed by the quantum memory channel whose action depends on the state evolution \(\varrho(t)\) (see, e.g., Ref. [31]). Other non-Markovian processes of Rabi oscillation damping in driven quantum dots are considered in Ref. [32].

For the sake of simplicity, we assume a point-like character of localized wavefunctions \(\ket{L} = (\ket{0} + \ket{1})/\sqrt{2}\) and \(\ket{R} = (\ket{0} - \ket{1})/\sqrt{2}\) in the left and the right dot in Fig. 1, respectively, i.e., \(a = d\). Taking into account the image charge potential (1), the Hamiltonian \(H\) in the basis of states \(\ket{0}, \ket{1}\) is

\[
H = \begin{pmatrix}
0 & 0 \\
0 & \hbar f
\end{pmatrix} - \frac{e^2}{2\hbar}(\varrho_{10} + \varrho_{11}) \left( \frac{1}{2D^2} + \frac{1}{4D^2 + d^2} \right) \begin{pmatrix}
0 & 1 \\
1 & 0
\end{pmatrix}.
\]

(22)

Substituting (21) and (22) in (20) and writing the latter equation in terms of dimensionless time \(t' = \hbar dt\), we obtain

\[
\frac{d}{dt'} \left( \varrho_{01} - \varrho_{11} \right) = -\left( \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \varrho_{10} \right) - iK(\varrho_{01} + \varrho_{10}) \left( \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \varrho_{11} - \varrho_{01} \right) - \frac{1}{Q \hbar f} \varrho_{11} \varrho_{01} \left( \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \varrho_{01} - \varrho_{11} \right).
\]

(23)

where by \(K\) we denote a ratio of the characteristic energy shift due image charge potential to the energy of qubit oscillations

\[
K = \frac{e^2}{2\hbar f} \left( \frac{1}{2D} + \frac{1}{4D^2 + d^2} \right) \approx \frac{e^2 d^2}{32 \hbar fD}\Omega^2
\]

(24)

To solve the system of differential equations (23) is a challenge (even numerically) so we exploit a small-parameter expansion, where the role of small parameter is played by \(1/Q\). Then one can replace the derivative \(d(\varrho_{01} + \varrho_{10})/dt\) by \(-i(\varrho_{01} - \varrho_{10})\). After this is done, it is convenient to describe the density matrix \(\rho\) by a real Bloch vector \(\lambda = (\lambda_x, \lambda_y, \lambda_z)\) defined through \(\rho = \frac{1}{2}(1 + \lambda \cdot \sigma)\), where \(\lambda\) is the identity matrix and \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) is a set of Pauli matrices. Then the system (23) yields the following dynamics of the Bloch vector:

\[
\frac{d\lambda_x}{dt} = -\lambda_y - \frac{2}{Q} \lambda_y \lambda_z
\]

(25)

\[
\frac{d\lambda_y}{dt} = \lambda_z + 2K\lambda_x\lambda_z - \frac{2}{Q} \lambda_y
\]

(26)

\[
\frac{d\lambda_z}{dt} = -2K\lambda_x\lambda_y - \frac{2}{Q} \lambda_z(1 + \lambda_z)
\]

(27)

The obtained system is readily solved numerically and examples are illustrated in Fig. 4. Interaction with the environment leads to dissipation and to a loss of quantum coherence (Fig. 4a). In Fig. 4b we take into account reservoir memory effects related with the image-force potential. At some times, these effects reverse the dissipative process and allow the qubit to regain some information and energy.
5. Summary

In summary, we have estimated the decoherence rate of charge qubits caused by energy loss in nearby electrodes. We have also considered the effect of decoherence and image-force potential on time evolution of the qubit. For realistic gate-engineered qubits, the quality of Rabi oscillations is shown to be \( Q = 40 \). The effect of image charge potential: (a) \( K = 0 \) and (b) \( K = 0.4 \).

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