Manipulations with qubit states by short control pulses: the interpolation method for evolution operator and fidelity

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Abstract. In this article the dynamics of the qubits states based on solution of the time-dependent Schrödinger equation is investigated. Using the Magnus method we obtain an explicit interpolation representation for the propagator, which allows to find wave function at an arbitrary time. To illustrate the effectiveness of the approach, the population of the levels a single and two coupled qubits have been calculated by applying the Magnus propagator and the result have been compared with the numerical solution of the Schrödinger equation. As a measure of the approximation of the wave function, we calculate fidelity, which indicates proximity when the exact and approximate evolution operator acts on the initial state. We discuss the possibility of extending the developed methods to multi-qubits system, when high-speed calculation methods of the operators of evolution is particularly relevant.

1. Introduction
Accurate and efficient solution of the time-dependent Schrödinger equation is important in the fields of the computational physics. In many situations, especially in the area of manipulating with quantum states of quantum bits (qubits), the evolution of the wavefunction occurs over multiple states and timescales, and a computationally efficient approach is a necessity for any progress. Simulation of qubits dynamics is important to obtain a fundamental understanding of “read-write” processes and to provide a theoretical base for the design and development of quantum gates for the optimal control over quantum registers [1, 2].

The numerical solution of the time-dependent Schrödinger equation for multilevel systems relies heavily on the discretization of the time-variable and to use standard methods of solutions of Cauchy problem for the differential equations with an initial value for wave function. The grid methods are usually used to find the evaluation operator (propagator) numerically, for instance, by applying the iterative methods, the method of fast-Fourier transformation, Crank-Nicolson methods and so on.

Another approach is based on composition of a suitable operator approximation when the propagator may be found explicitly at an arbitrary moment. In the case of a time-independent Hamiltonian the most popular long-time propagator is Chebyshev polynomial propagator [3]. It is
accomplished as follows: the propagator at the first decomposed into Chebyshev polynomials, which are then computed using iterative procedures.

When the Hamiltonian is time-dependent, such as in a case where propagating ultra-short pulse acts on an array of qubits [4-7] the efficiency of the evolving methods of the propagator is crucial for computer modeling of the quantum dynamics. In the present work, the Magnus expansion method for propagator will be presented. Using this method we will obtain a convenient representation for the evolution operator, which makes it possible to find an explicit expression for the propagator at any time. To illustrate the effectiveness of the approach, the populations of the levels a single and two coupled qubits at an arbitrary time will be calculated and compared with the numerical solution of the Schrödinger equation. As a measure of the approximation of the wave function, we calculate fidelity, a value that indicates proximity when the exact and approximate evolution operator acts on the initial state. In conclusion, we will discuss the possibility of extending the developed methodology to multi-qubit systems, where high-speed calculation methods are particularly relevant for evolution operators.

### 2. The model of the system and the basic equations

The Hamiltonian of the superconducting flux qubit [8] can be represented as

$$H(t) = \hbar (\Delta \sigma_z + \varepsilon(t) \sigma_x),$$

where $\hbar \Delta$ is the distance between qubit levels; $\varepsilon(t)$ is the control function (proportional to the magnetic flux); $\sigma_z, \sigma_x$ are Pauli matrices. When $\varepsilon = 0$ the solution of the time-nondependent Schrödinger equation has the form: $\psi_0(t) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$. $E_0 = -\hbar \Delta / 2$ and $\psi_1(t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. $E_1 = \hbar \Delta / 2$, which corresponds to the choice of the two qubits levels with energies $E_0$ and $E_1$. We are interested in the processes of switching of the qubit from one basic state to another under the impact of an unipolar external pulse $\varepsilon(t) = \varepsilon_m \exp(-(t-t_0)^2 / 2\tau^2)$ (where $\varepsilon_m$ is the pulse amplitude; $\tau$ is the typical pulse duration and it is supposed to be $t_0 \gg \tau$ for a gaussian pulse). The time dependence of the two-component wave function of a qubit is determined by: $\psi(t) = U(t)\psi(0)$, where $\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is wave function of ground qubit state at the initial time, the propagator $U(t)$ is the evolution operator, $U(0) = I, U^\dagger = U^{-1}$ is the solution of the equation

$$i\hbar \frac{dU(t)}{dt} = H(t)U(t).$$

The solution of the Eq. (2) can be written in the form: $U(t) = \hat{P}\exp\left(-\frac{i}{\hbar} \int_0^t dt_t H(t_t)\right)$, where $\hat{P}$ is chronological ordering operator. The exact solution of Eq. (2) is found by a numerical solution Eq. (2) of the system of equations obtained when the operator is parameterized in a certain basis.

In this paper we develop a technique for calculation of the operator Eq. (2) based on the construction of approximate representation of the evolution operator – Magnus expansion. The essence of the method is the following. At the first, the evolution operator can be represented in the form of: $U(t) = e^{A(t)}$, where $A(t)$ the anti-Hermitian operator. According to [9], the operator $A(t)$ is expanded in the series, where the terms are proportional to the corresponding degrees of the Hamiltonian operator: $A_m = A_1 + A_2 + A_3 + \ldots$. This decomposition is substituted in Eq. (2). The resulting equality for the corresponding components of the same order of smallness on the left and the right, which leads to the ratios:
\[ A_1(t) = -\frac{i}{\hbar} \int_0^t dt_1 H(t_1), \quad A_2(t) = \frac{1}{2\hbar^2} \int_0^t dt_2 \int_0^{t_1} dt_1 \left( [H(t_1), H(t_2)] + \frac{A_2(t)}{3} \right). \]

If there is a small parameter in the system, we can keep only several terms in the series of the Magnus expansion.

However, the resulting expression for \( U_M(t) = e^{A_4(t)} \) is difficult to use in practice, because we need to take action on the state of the operator in the exponent of the exponential. Further the idea that we can lead the term \( A_3(t) \) in time \( t \) to the expression \( A_4(t) = V(t)D(t)V(t) \) (where \( D(t) \) is a diagonal matrix, \( V(t)V(t) = I \)), and then to use the relation: \( U_M(t) = e^{V(t)D(t)V(t)} = V(t)e^{D(t)V(t)} \).

For a two-level system – qubit – the Hermitian operator can be written in the form \( \hat{A} = -i\hat{T} \) (\( \hat{T}^\dagger = \hat{T} = T_x \sigma_x + T_y \sigma_y + T_z \sigma_z \)). For the two-component wave function the evolution operator \( U_M \) can be written as follows:

\[ U_M = \cos T\left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) - \frac{i\sin T}{T} \left( \begin{array}{cc} T_x & T_x + iT_y \\ T_x - iT_y & -T_x \end{array} \right), \]

where time-dependent functions \( T_x(t), T_y(t), T_z(t) \) are determined by the expressions:

\[ T_x + iT_y = \int_0^t dt_1 \epsilon(t_1) e^{-it_1}, \quad T_z = \frac{1}{2} \int_0^t dt_2 \epsilon(t_2) \frac{\hbar}{\hbar} \epsilon(t_2) \sin(\Delta t - t_2). \]

The eigenvalues of anti-Hermitian operator \( \hat{T} \) are equal to \( \pm T \), where \( T = \sqrt{T_x^2 + T_y^2 + T_z^2} \).

Thus, the qubit evolution procedure is reduced to constructing the matrix \( U_M \) according to the Eq. (4) and further by calculating the wave function by using a simple rotation in the "pseudospin" space of the qubit as: \( \psi(t) = U_M(t)\psi(0) \). As a criterion of proximity matrices one can take various measures matrix characterizing the proximity matrices \( U(t) \) and \( U_M(t) \). For the "write-read" quantum information tasks it’s advisable to choose a measure (fidelity \( F(t) \)) defined by the wave functions \( \psi(t) \) and \( \psi_M(t) \) at the current time according to:

\[ F(t) = \left| \left< \psi(0) \right| U_M(t)U(t) \left| \psi(0) \right> \right|^2. \]

When \( F(t) = 1 \) during the evaluation the both the states are the same and we have a good approximation for propagator.

### 3. The populations and fidelity calculation for qubit

Now we shall demonstrate that the developed technique allows us to select analytically and numerically the optimal form of a single quantum pulse. For comparison of these two solutions, we follow the time changes in the probability of population of the qubit excited state under the action of the gaussian pulse with a given amplitude \( \epsilon_m \) and duration \( \tau \). The qubit initialized (at the \( t = 0 \)) to the ground state \( \psi_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \), \( \epsilon_0 = -\frac{\hbar\Delta}{2} \) and we are calculated the probability of state switching.
\( \psi_0 \to \psi_1 \), respectively \( p(t) = \left| \langle \psi_1 | \psi(t) \rangle \right|^2 \), \( p_M(t) = \left| \langle \psi_1 | \psi_M(t) \rangle \right|^2 \). Analyzing the expression (4) it is possible to notice, that \( \Delta \tau \ll 1 \) is the criterion for good convergence of analytics and numerical calculation [1]. Figure 1 (a) demonstrates the behavior of the qubit ground state population at different tunneling energies \( \Delta \). Note that a solution based on the construction of approximate representation of the evolution operator – Magnus expansion (dashed red curve \( \Delta \tau \parallel 0.15 \)) agrees well with the numerical calculations (solid red curve), while fidelity after unipolar pulse is \( F = 0.99995 \) (red curve in figure 1 b). The increase in the tunneling energy of the qubit leads to divergence of the solutions (see figure 1 b). When going beyond the conditions \( \Delta \tau \ll 1 \) for a more accurate analytical expression (4) it is necessary to consider more terms of the expansion in Eq. (3).

\[ H(t) = -\frac{\hbar}{2} \begin{pmatrix} 2\varepsilon(t) + J & \sqrt{2}\Delta & 0 \\ \sqrt{2}\Delta & -J & \sqrt{2}\Delta \\ 0 & \sqrt{2}\Delta & -2\varepsilon(t) + J \end{pmatrix}. \]  

Figure 1 (a) The results of numerical (solid curves) and analytical (dashed curves) calculations for the time-dependent population probabilities \( p(t) \) and \( p_M(t) \) of the qubit ground state and (b) the matching fidelity \( F(t) \) of the numerical and analytical solutions at different tunneling energies of the qubit. Red curves – \( \Delta = 0.05 \) GHz, blue curves – \( \Delta = 0.1 \) GHz, green – \( \Delta = 0.25 \) GHz and black curves – \( \Delta = 0.5 \) GHz. The pulse parameters used here are: \( \tau = 3 \) ps, \( t_0 = 1 \) ps, \( \varepsilon_m = 0.65 \) GHz.

4. Multi-qubits systems
We have considered also the problem of controlling the populations of two qubits under the influence of a Gaussian pulse. The most interesting situation arises in the case when their parameters coincide, and control is carried out by the same impulse [10]. For identical qubits, the wave function can be decomposed into two orthogonal states: a singlet (scalar) and a triplet (vector).

\[ H(t) = -\frac{\hbar}{2} \begin{pmatrix} 2\varepsilon(t) + J & \sqrt{2}\Delta & 0 \\ \sqrt{2}\Delta & -J & \sqrt{2}\Delta \\ 0 & \sqrt{2}\Delta & -2\varepsilon(t) + J \end{pmatrix}. \]  

When the control parameter \( \varepsilon = 0 \), there are three levels of coupled symmetric qubits: \( \{-\hbar \sqrt{(J/2)^2 + \Delta^2}, -\hbar J/2, \hbar \sqrt{(J/2)^2 + \Delta^2} \} \). Time dependent external field will lead to transitions between them. For example, if a state with a lower energy is initially populated, then it is possible to raise the question of preparing the given populations of the remaining levels.

The interpolation evolution operator for a given system is constructed according to the scheme described above. We give an explicit expression for the case when the terms \( \sim \Delta \) are taken into account in the exponent:
\[ U_{st} = \frac{1}{T^2} \begin{pmatrix} 
 e^{-iT} |\xi|^2 + |\eta|^2 & 0 & -2ie^{-iT/2} \xi \eta \sin(T/2) \\
 0 & T^2 e^{-iT} & 0 \\
 -2ie^{-iT/2} \xi^* \eta^* \sin(T/2) & 0 & |\xi|^2 + e^{-iT} |\eta|^2 
\end{pmatrix}, \tag{8} \]

where \( \xi(t) \) and \( \eta(t) \) are the functions of time:

\[ \xi(t) = -\frac{\Delta}{\sqrt{2}} \int_0^t dt_i \exp(iJt_i + i\int_0^{t_i} dt_j \varepsilon(t_j)) \quad \text{and} \quad \eta(t) = -\frac{\Delta}{\sqrt{2}} \int_0^t dt_i \exp(-iJt_i + i\int_0^{t_i} dt_j \varepsilon(t_j)) , \]

and \( T(t) = \sqrt{|\xi(t)|^2 + |\eta(t)|^2} \). The level populations for the selected values of the qubit parameters, calculated according to (8), for the chosen parameters only qualitatively agree with the exact numerical solution of the Schrödinger equation (see Fig. 2).

**Figure 2** The results of numerical \( p_i(t) \) (a) and analytical \( p_{i,\text{ap}}(t) \) (b) calculations for the time-dependent population probabilities of a pair of symmetric qubits: \( J = 0.05 \text{ GHz} \), \( \Delta = 0.05 \text{ GHz} \), \( \varepsilon_m = 1 \text{ GHz} \), \( \tau = 3 \text{ ps} \), \( t_0 = 1 \text{ ps} \). The red curve corresponds to population of ground state; the blue and black lines depict the populations of the second and the third levels.

Analyzing the data we arrive to the conclusion that for multi-qubits systems it may be necessary to take into account the neglected terms in the expansion (3).

5. **Conclusion**

We have developed here the interpolation method of approximation the evaluation operator of a multi-qubits system with a time-dependent Hamiltonian. To calculate the propagator system the Magnus expansion for the evolution operator has been applied, which makes it possible to find an explicit expression for the wave function at any time. The effectiveness of the approach has been illustrated by the calculation of the levels populations of a single and two coupled qubits and by comparing with the results with the numerical solution of the Schrödinger equation. We have investigated the fidelity which is playing role of the convenient measure of the approximation and that is indicated proximity when the exact and approximate evolution operator acts on the initial state. The carried out analytical and numerical simulations have demonstrated the possibility of accelerating the numerical solution of evolutionary problems by the developed method.

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