Design of Adiabatic Logic for a Quantum CNOT Gate

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We examine the realization of a quantum CNOT gate by adiabatic operations. The principles of such systems and their analysis are briefly discussed and a model consisting of two weakly coupled double-potential well qubits is studied numerically. Regions of the parameter space with suitable well-defined sets of wavefunctions are found, in which then an adiabatic sweep of an external bias produces the switching behavior of CNOT. Results are presented on the adiabatic condition and the identification with the parameters of a flux-coupled two-SQUID system is given. For typical parameters adiabatic times in the nanosecond regime are obtained.

The basic element of the “quantum computer” [1] is the quantum bit (qubit), a two level system, exhibiting quantum coherence between the states. Many physical realizations of the qubit have been proposed [2]. To manipulate the qubit quantum gates [3] are necessary, logic devices capable of operating on linear combinations of input states. First there is the simple NOT, a one bit operation which can be viewed as an inversion operation on a qubit. The next step is to construct gates of a conditional character. A simple case to consider is the two-bit operation “controlled NOT” or CNOT. To realize such device it is natural to consider using an interaction between the physical elements constituting the qubit.

Among the possible mechanisms for manipulating coupled qubits adiabatic procedures are, as explained below, of special interest. Furthermore, it has been suggested that adiabatic procedures may be robust with respect to certain kinds of errors [4]. In particular with superconducting devices, Averin [5] has suggested using small Josephson junctions in the Coulomb blockade regime, and we have mentioned the possibility of using SQUID qubits with flux coupling [6]. In this letter we will explain some general principles for studying such systems and to present numerical calculations relevant to their behavior and design.

CNOT is a two-qubit operation and we will represent it by two interacting double-potential well systems. Each double well system may be thought of as an approximately independent qubit since we shall keep the coupling weak. Qualitatively, we will use the procedure of performing an adiabatic NOT [6] on the first qubit while trying to influence its behavior by the state of the second. We find a region of parameter space where this works.

Hamiltonian: We take the following model Hamiltonian

$$H = \frac{-1}{2\mu_1} \partial^2 \phi_1^0 + \phi_1^0 + \frac{-1}{2\mu_2} \partial^2 \phi_2^0 + V$$ (1)

containing dimensionless “masses” $\mu$ and dimensionless “position” coordinates $\phi_1, \phi_2$, while the potential term is

$$V = V_0 \left\{ \frac{1}{2} [l_1 (\phi_1 - \phi_1^{ext})^2 + l_2 (\phi_2 - \phi_2^{ext})^2] + 2 l_1 (\phi_1 - \phi_1^{ext})(\phi_2 - \phi_2^{ext}) \right\} + \beta_1 f(\phi_1) + \beta_2 f(\phi_2).$$ (2)

The function $f(\phi)$ is chosen so that a double-well potential results for each $\phi$ variable. We shall use $f(\phi) = 1 - \frac{1}{2} \phi^2 + \frac{1}{4} \phi^4$. $V_0$, $l_1$, $l_2$, $l_12$, $\beta_1$ and $\beta_2$ are constants depending on system parameters. The two $\phi^{ext}$ are external biases which can be adjusted or varied to perform the operation and find favorable operating points for the device. Their values determine the degree of asymmetry of each double well system; when they are zero the wells are symmetric (for $l_12 = 0$). Note that when the coupling parameter $l_12$ is zero the hamiltonian simply represents two non-interacting systems. Our model system thus consists of two weakly interacting double-potential wells with externally adjustable biases $\phi_1^{ext}, \phi_2^{ext}$. Fig 1 shows the equipotential contours of $V(\phi_1, \phi_2)$, with its four potential wells.

Representation of Logical States: We first require a representation of the four states of the two-qubit system.
Each logical state will be represented by a wavefunction localized in a distinct potential well. When this obtains, the logical state corresponds to a distinguishable physical state with high probability. With SQUID qubits, for example, if for a single SQUID a wavefunction concentrated on the left of the double potential well corresponds to current going clockwise, then for a two-SQUID system the lower left well of Fig 1 corresponds to current counter-clockwise in SQUID 2 and current clockwise in SQUID 1. Since, as will be explained in the next paragraph, we work with energy eigenstates, a first requirement on the hamiltonian is thus that it yield a set of “good wavefunctions”, that is where the first four energy eigenstates are well localized in the four different wells of Fig 1.

Assuming such a set of wavefunctions has been found, visualization of the situation is aided by the use of tableaux indicating where the wavefunctions are localized on Fig 1. Labeling the first four energy eigenstates in order of increasing energy 1, 2, 3, 4, examples of possible tableaux are seen in Eq[3].

**Representation of CNOT:** Our aim is to represent a logical operation such as CNOT by a mapping of the set of initial logical states to a certain set of final logical states. This will be represented by a particular rearrangement of states on the tableau.

CNOT is defined by the conditions: A) the control bit does not change its state, and B) the target bit is reversed or not reversed, according to whether the control bit is 1 or 0. If we identify the top row of the tableau with control bit =0 and the bottom row with control bit = 1, a physical embodiment of CNOT would be

\[
\begin{pmatrix}
4 & 3 \\
1 & 2
\end{pmatrix} \rightarrow 
\begin{pmatrix}
4 & 3 \\
2 & 1
\end{pmatrix},
\]  
(3)

Condition A) on the stability of the control bit is exhibited in that no states move between the top and bottom row. Condition B) is realized in that the top row remains unchanged while the bottom row is “flipped”.

**Adiabatic Operations:** Realization of operations such as Eq[3] can be accomplished in an especially transparent way by using adiabatic processes. This is due to the “no level crossing” behavior of adiabatic evolution. The no-crossing property assures that a state initially in the first, or second, or third,... energy level after the adiabatic evolution, while at the same time the physical properties associated with the level may be changing. Thus in Eq[3] with SQUIDs, state 1 begins as a configuration with the current clockwise in SQUID 1, counter-clockwise in SQUID 2 and ends up as a configuration where the current remains counter-clockwise in SQUID 2 but is now reversed to counter-clockwise in SQUID 1.

One can proceed as follows: we search for an initial hamiltonian whose variable parameters \((\psi^0, \phi^0)\) are adjusted to give the left tableau of Eq[3]. Then, we search for a final hamiltonian where another set of \((\psi^f, \phi^f)\), gives the tableau on the right. If the two parameter sets can be connected by a smooth, slow transformation,-a “sweep”- we have obtained an adiabatic realization of our operation, here CNOT.

In this procedure we need only to study the stationary Schroedinger equation at first. This is an important simplification for the numerical analysis. However, after having determined some suitable parameter sets we shall also study the full time-dependent Schroedinger equation. This is necessary to determine what sweep speed is “slow”, that is guarantees adiabatic behavior.

**Numerical Methods:** Our problem involves two variables and tunneling through four barriers, as well as a multi-dimensional parameter space. To deal with this complex situation we turn to a recently developed method [7] for numerical solution of the Schroedinger equation. A large basis of harmonic oscillator wavefunctions is used to reduce the problem to an array of fast algebraic manipulations, programmed in Mathematica. Except for the small \(l_{12} \sim 10^{-3}\), we work with parameters of order one, hence the resulting dimensionless energies are also of order one. However the splittings among the lowest levels, which are what we manipulate, result from tunneling and are small \(10^{-3-}\sim 10^{-4}\). Hence four place accuracy is necessary. Using these methods we have been able to find a region of the \((\phi^0, \phi^f)\) parameters space where there are “good wavefunctions”. These are indicated as the gray regions of Fig 2, with the parameters as indicated. Reducing the value of \(l_{12}\) leads to a shrinking of these regions on the plot.

As a by-product of our numerical work we can also examine the validity of the frequently used “pseudo-spin” picture. One often usefully visualizes [6] the lowest quasi-degenerate levels of the system as “spins”. This picture requires, however, that the moving statevectors remain in the hilbert space spanned by an initial (here four) set of states. By evaluating wavefunction overlaps we find this is true, to a good approximation, supporting the use of the “spin” picture. We stress, however, that we do not need this simplification in our calculations.

**Switching Behavior:** We have been able to obtain switching behavior according to Eq[3] for the “good” regions of Fig 2, by means of the following operation: the control bias \(\phi^f\) is held constant at a relatively high value while there is a sweep of the target bias \(\phi^i\). This is a generalization of a simple NOT [6] on \(\phi^i\). The results
may be understood in terms of a simple model: the $l_{12}$ coupling produces an extra bias on the target bit which "helps or hinders" the NOT operation.

The relatively large bias on $\phi_2$ comes from condition A): we attempt to "immobilize" the control bit despite the perturbations communicated by the sweep of $|\phi_2|$. We therefore investigate the region $|\phi_2| < |\phi_{ext}|$. If $\phi_2$ is indeed successfully "immobilized" it will be fixed in one of its two potential wells and can only have the values $\phi_2 \approx \pm 1$. As seen by $\phi_1$, this amounts to $\pm$ an extra bias. To linear order (since we take all $\phi_{ext}$ small compared to 1 and $\phi_1, \phi_2$ are in the neighborhood of 1) and introducing the notation

$$\phi_{ext}^1 = \phi_{ext} \pm \frac{l_{12}}{l_1}$$

the potential terms involving $\phi_1$ in Eq [2] become

$$-2l_1\phi_1\phi_{ext}^1 - 2l_{12}\phi_1(\pm 1) = -2l_1\phi_1(\phi_{ext}^1 \pm \frac{l_{12}}{l_1}) = -2l_1\phi_1\phi_{ext}^{1\ eff \ f} ,$$

As a consequence, there is an effective shift in the external bias on $\phi_1$ by $(\pm \frac{l_{12}}{l_1})$. This is just as suggested by the "help or hindering" picture, and we further learn that the magnitude of the "help" is $\frac{1}{l_1}$. According to this picture we should try to analyze the behavior of $\phi_1$ (target bit) as if it were simply under a modified external bias $\phi_{ext}^{1\ eff \ f}$.

We would then expect if a certain tableau obtains and $\phi_{ext}^1$ is varied, that the tableau is maintained until there is a sign switch for $\phi_{ext}^{1\ eff \ f}$. To see how the sign switch occurs, note that for $\phi_{ext}^1 \approx 0$ the sign of $\phi_{ext}^{1\ eff \ f}$ is given by the $\pm$ from the control bit. But for $|\phi_{ext}^1| >> \frac{l_{12}}{l_1}$, the sign is controlled by $\phi_{ext}^1$ itself. There is, therefore, a region around $\phi_{ext}^1 = 0$ where the tableau is determined by the control bit, and another region for large $|\phi_{ext}^1|$ where the tableau is determined by the sign of $\phi_{ext}^1$. As we cross from one region to another, one pair of states will retain the sign it had for large $|\phi_{ext}^1|$ and the other pair of states will switch. This would be the desired behavior. According to Eq [4] the point where the switch from one tableau to another should take place is given by $|\phi_{ext}^1| \approx \frac{l_{12}}{l_1}$.

**Numerical Results:** The three different gray areas of Fig 2 have well defined tableaux as follows:

$$\begin{pmatrix} 3 & 4 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 4 & 3 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} 4 & 3 \\ 2 & 1 \end{pmatrix}$$

for the intermediate gray region (left), the darkest region (center) and the light gray region (right), respectively. These tableaux fit with the description arrived at in the model, where either the top or bottom row inverts as we go from the central region to large $|\phi_{ext}^1|$. Hence a sweep from the central region to the right region produces the mapping Eq [3]. Similarly sweeping from the right region to the center and from the left region to the central region and vice-versa can also serve as realizations, differing simply in the assignment of (0,1) for the quantum states or the names for the qubits. Fig 2 shows that the switch between tableaux occurs quite close to $|\phi_{ext}^1| = |l_{12}/l_1|$, as predicted by the model. Also, it seems the inequality $|\phi_{ext}^1| << |\phi_2|$ need not be very strong for "immobilization".

**Adiabatic Condition:** An important time scale is $\tau_{adiab}$, the shortest time in which an operation can be performed adiabatically. This time is relevant both to the maximum speed of the device and with respect to decoherence and relaxation effects since the operation must take place in times short compared to those for these effects. We thus now examine the *time dependent* Schroedinger equation $i \frac{\partial \psi}{\partial t} = H \psi$. We work with the dimensionless time variable $\tau$, where the connection to usual time $t$ is given by $\tau = E_0 t$. $E_0$ is an energy parameter in electron volts or Hz, characteristic of the particular system under consideration. It also gives the overall energy scale. Thus all energies are in units of $E_0$ and all times are in units of $E_0^{-1} (\hbar = 1)$.

An estimate for NOT [6] gave

$$\tau_{adiab} = \frac{\omega_{tunnel}^2}{\epsilon} = \epsilon \tau_{rabi}^2 ,$$

where $\epsilon$ is the length of the sweep in energy and $\omega_{tunnel}^{-1} = \tau_{rabi}$, the inverse tunneling energy or oscillation time between the two states at minimum separation. Since here we also perform a kind of NOT, we expect a similar relation to hold, where $\omega_{tunnel}$ or $\tau_{rabi}$ is the smallest level splitting during the adiabatic passage and the sweep length $\epsilon$ may be read off from the total energy shift of the wells. We define a "degree of adiabaticity" by performing a sweep numerically and taking the overlap of the resulting wavefunction with the wavefunction of the corresponding stationary final Hamiltonian; that is to say the overlap with the wavefunction that would result from an infinitely slow sweep. The square of this amplitude, $P_f$, is shown in Fig 3 as a function of sweep time, for a sweep (0.002, −0.01) → (0.008, −0.01) on Fig 2. The arrow indicates the theoretical prediction using Eq[7]. As would be expected, $\tau_{adiab} \approx \epsilon^{5.2} \approx 500$ is a large number in dimensionless units.

**Identification with SQUID parameters:** Eqns [1,2] arise by standard methods in the analysis of two rf SQUID loops coupled by an mutual inductance $L_{12}$ [8]. The Josephson relation leads to $f(\phi) = \cos \phi$, to which our $f(\phi) = 1 - \frac{1}{2} \phi^2 + \frac{3}{4} \phi^4$ is a good approximation.

With $L_1, L_2$ the SQUID inductances and $C_1, C_2$ the Josephson junction capacitancies, the energy scale factor is $E_0 = 1/\sqrt{LC}$, where $C = \sqrt{C_1 C_2}$ and $L = L_{12} - L_{12}^2 \approx \sqrt{L_1 L_2}$. A set of reasonable values for the SQUID is $L_1 = 300 pH$, $L_2 = 250 pH$, $L_{12} = 1.8pH$, $C_1 = C_2 = 0.1 pF$ and $\beta_1 = \beta_2 = 1.28$. Since in frequency units one finds $E_0 \approx \frac{1}{\sqrt{L_{ph} C_{ph} F}} \approx 1000$ GHZ these values give $E_0 \approx 185$ GHZ. Then the $\tau_{adiab} \approx 500$ in dimensionless units.
FIG. 2. A region of the $\phi_{1}^{ext}, \phi_{2}^{ext}$ plane with a well defined set of wavefunctions as explained in the text. The coupling parameter is $l_{12} = 0.005$. Other parameters were $l_{1} = l_{2} = 1$, $\beta_{1} = \beta_{2} = 1.19$, $\mu_{1} = \mu_{2} = V_{0} = 16.3$.

FIG. 3. The adiabaticity parameter versus sweep time for a sweep of $(\phi_{1}^{ext}, \phi_{2}^{ext}): (0.002, -0.01) \rightarrow (0.008, -0.01)$. $P_{fi}=1$ denotes perfect adiabicity. The arrow indicates the theoretical estimate $\tau_{adiab} = \epsilon \omega_{tunnel}^{-2}$. Units corresponds to $\tau_{adiab} \approx 500/E_{0} \approx 2.7 \cdot 10^{-9}$s in seconds.

Finally we note that here, as with all discussions of quantum computation, the important open question is the time scale for decoherence $\tau_{dec}$. In [6] we estimated $\tau_{dec} \approx (few) \times 10^{-6}$s for the SQUID at 40mK (and also suggested a method for its direct measurement). With the above estimate for $\tau_{adiab}$ it thus appears, at least for the SQUID, that the adiabatic condition allows for operations in times less than $\tau_{dec}$. However, the question of the decoherence time is controversial and system-dependent and will probably only be resolved convincingly by experiment. In this respect, it is encouraging that in experiments [9] showing evidence for macroscopic quantum behaviour of the SQUID the dissipation value is rather small.

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