Quantum gates using a pulsed bias scheme

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We propose a scheme for realizing quantum gates [controlled-NOT (CNOT) and Toffoli] using a two-level quantum system by means of a pulsed bias. We show how to realize a CNOT gate using a two-qubit, two-level coupled system and a Toffoli gate using a three-qubit, two-level coupled system. For the CNOT gate, we show how to reduce the 4×4 Hamiltonian of the coupled system to a 2×2 Hamiltonian in order to solve for parameter values of the system. When these values are substituted into the coupled system equations for the two-qubit system, the simulation results confirm the CNOT gate operation. We further demonstrate our proposed scheme for a CNOT gate operation using a multilevel system of two coupled superconducting quantum interference devices as a particular example. We next use the same approach to implement a Toffoli gate using a three-qubit system.

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I. INTRODUCTION

It has been shown that for universal quantum computing, any unitary operator can be generated if a means exists to achieve arbitrary single-qubit rotations, and one nontrivial two-qubit operation like a controlled-NOT (CNOT) [1–4]. In their paper, M. F. Bocko *et al.* [5] discuss the prospects and challenges for implementing a quantum computer using superconducting electronics. Methods have been proposed for realizing single-qubit operational gates with Josephson qubits [6–8] using microwaves. Recently, macroscopic quantum coherence between the two charge basis states of a superconducting charge qubit was demonstrated by Nakamura *et al.* [9], where it was shown how an arbitrary rotation can be realized by controlling the gate voltage. A conditional gate operation using two superconducting charge qubits has been demonstrated wherein the two-qubit solid-state circuit was controlled by means of a pulsed technique [10]. In Ref. [10], Yamamoto *et al.* used a pulse technique to demonstrate conditional gate operation using a pair of superconducting charge qubits in which they brought their system to a degeneracy point or a virtually nonoscillatory point depending on the state of the control qubit. In Ref. [11], Strauch *et al.* show how to realize a phase gate and a swap-like gate in a capacitively coupled Josephson junction system by varying bias currents with time, through a detuning parameter. A two-qubit phase gate using a quantum interference scheme requiring three symmetric steps where the tunneling is controlled by varying the height of the potential barrier for set intervals of time has been proposed by Charron *et al.* [12]. In Ref. [13], Benjamin *et al.* show how a system with a constant coupling can be employed for quantum computing by actively tuning the transition energies of individual qubits.

Our scheme is similar to Ref. [10] in that we reduce the system into a two-level system with two different Hamiltonians depending upon the state of the control qubit A. The scheme in Ref. [10] uses a pulsed bias to either bring the system to a degeneracy point, where it oscillates between the $|00\rangle$ and $|01\rangle$ states, or to a nonoscillatory point far from the degeneracy point of the $|10\rangle$ and $|11\rangle$ states. A sufficiently strong coupling ensures that the $|10\rangle$ (or $|11\rangle$) state remains unchanged. In our scheme, we use a weak coupling such that when the bias is pulsed low, it either completely cancels the coupling or adds to it giving rise to two frequencies of oscillation, one between the $|00\rangle$ and $|01\rangle$ states and the other between the $|10\rangle$ and $|11\rangle$ states. By reducing the 4×4 Hamiltonian matrix of the coupled system to a 2×2 matrix, we solve for parameter values of the system in order to achieve a CNOT gate operation by controlling these two frequencies. We also show that these parameters can be scaled, where the limits on the parameter values are those imposed by experimental conditions. This means that having found the parameter values for a pulse width of certain duration, the parameters for a different pulse width are just a multiple of the original values (the multiple depends on the ratio of the two pulse widths under consideration).

Not only is the CNOT gate, in addition to single bit rotations, sufficient to perform all logic operations within a quantum computer, but it can also be used to construct arbitrary unitary transformations on any finite set of bits [2,14–19]. Proposals have been made for constructing the Toffoli gate [4], which is the smallest reversible quantum gate, using the CNOT gate and some single-qubit gates. The Toffoli gate requires three inputs and has three outputs. Even though this corresponds to a quantum mechanical scattering process involving three-particle collisions [17], the Toffoli gate can be constructed by two-particle scattering processes [2,3,18,19]. In this paper, we extend our pulsed bias scheme for realizing this gate using a three-qubit, two-level system. Two of the qubits behave as controls, whereas, the third qubit behaves as the target and flips its state only when both of the control qubits are in the $|1\rangle$ state. The target qubit is weakly coupled to both the controls, which are not directly coupled to each other. Like the CNOT, the state of the target changes during a pulse of its bias. An approach for calculating the parameter values to achieve the gate operation will be presented in this paper.

The gate implementation techniques using a pulsed bias scheme as described in this paper can, in general, be used for any two-level quantum system whose Hamiltonian can be reduced to that of a spin boson. In this paper, we show how to derive formulae for calculating the values of parameters related to the quantum system in order to realize the desired gate operations. Reducing the 4×4 Hamiltonian to a 2×2 effective Hamiltonian to calculate parameter values for the desired gate operation works well, not only for qubits of two-level systems (which are difficult to find among solid-state systems), but, in principle, for all qubits of multilevel systems as long as the other states are well separated from the four basis states in energy. Therefore, the method is relevant to the experiment.

II. COUPLED TWO-QUBIT SYSTEM

The four states of a two-qubit, two-level coupled system are $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$, where the first qubit represents the control A, and the second represents the target B. Here, $|0\rangle$ and $|1\rangle$ are the two basis states of a single-qubit, two-level system, given as,

$$|0\rangle = \begin{pmatrix}1\\0\end{pmatrix} \text{ and } |1\rangle = \begin{pmatrix}0\\1\end{pmatrix}.$$

The time evolution of the system is governed by the Schrödinger wave equation and the state of the system at any time is given as

$$|\psi(t)\rangle = \alpha(t)|00\rangle + \beta(t)|01\rangle + \gamma(t)|10\rangle + \delta(t)|11\rangle, \quad (1)$$

where $\alpha(t)$, $\beta(t)$, $\gamma(t)$, and $\delta(t)$ are the probability amplitudes representing the system in each of the four states, respectively.

The Hamiltonian of the system is given as

$$H = H_A + H_B + H_I, \quad (2)$$

where

$$H_A = \Delta_A\sigma_{XA} + \varepsilon_A\sigma_{ZA}, \quad H_B = \Delta_B\sigma_{XB} + \varepsilon_B\sigma_{ZB}, \quad (3)$$

and

$$H_I = \xi\sigma_{ZA}\sigma_{ZB}. \quad (4)$$

Here, H_A and H_B are the uncoupled Hamiltonians for qubits A and B, respectively, H_I is the interaction energy for the two qubits, ε_A and ε_B are the biases, Δ_A and Δ_B are half the uncoupled tunneling frequencies, ξ is the coupling factor, and σ_{XA}, σ_{ZA}, σ_{XB}, and σ_{ZB} are outer products of the Pauli matrices, σ_X and σ_Z, with the identity matrix for qubits A and B, respectively.

III. REDUCED HAMILTONIAN FOR THE CNOT GATE

In Ref. [9], Nakamura *et al.* reported the observation of quantum oscillations in a single Cooper-pair box and, thereby, demonstrated coherent control of a qubit in a solid-state electronic device by applying a short voltage pulse via a gate electrode. The resulting state, a quantum superposition of the two charge states, is detected through a probe junction where the current is proportional to the probability of the qubit being in the $|1\rangle$ state. In general, this effect can be extended to any two-level system whose Hamiltonian can be reduced to that of a spin boson. Such a system has the characteristic energy level anticrossing as one of the external control parameters (bias ε) is varied. Therefore, coherent control of the qubit can be achieved by pulsing the bias ε on and off. Starting with an arbitrary initial state, the probability of the qubit in the $|1\rangle$ state can be written as an oscillatory function in terms of the parameters Δ (tunneling) and ε (bias). Since we always prepare the system either in the $|0\rangle$ or $|1\rangle$ state, the probability function can be written as

$$P_{|1\rangle} = X \mp Y\cos(2\pi f t), \quad (5)$$

where the offset X, the amplitude Y, and the frequency f of probability oscillation are given as

$$X = \frac{1}{2} \mp \frac{\varepsilon^2}{2(\Delta^2+\varepsilon^2)}, \quad (6)$$

$$Y = \frac{\Delta^2}{2(\Delta^2+\varepsilon^2)}, \quad (7)$$

$$f = 2\sqrt{(\Delta^2+\varepsilon^2)}, \quad (8)$$

where the '$-$' and '$+$' are used when the qubit starts out in the $|0\rangle$ and $|1\rangle$ states, respectively, as its initial state. We have chosen units where Planck's constant is 1.

An arbitrary rotation can be realized for a single qubit by turning the bias ε on and off. When $\varepsilon \gg \Delta$, since the amplitude Y is very small and the offset X is either 0 or 1, depending on the initial conditions, the qubit remains in the state it has been initialized to and, hence, a *memory* state is realized. However, when the bias is turned off, i.e., $\varepsilon=0$, the qubit oscillates between the two basis states. We call this oscillatory state of the qubit a *transitional* state.

The controlled-NOT (CNOT) gate is defined by the following operator [20]:

$$\text{CNOT} = |00\rangle\langle 00| + |01\rangle\langle 01| + |10\rangle\langle 11| + |11\rangle\langle 10|. \quad (9)$$

To realize a CNOT gate from a coupled two-qubit system, the parameters of the governing Hamiltonian must be chosen such that starting out in an initial state, the system evolves into the desired state under the gate operation within a specified time interval. Unlike the dynamics of a single-qubit system, the time evolution of a two-qubit coupled system is governed by a 4×4 Hamiltonian matrix, which makes finding a closed-form equation similar to Eq. (5) for the probabilities in the $|1\rangle$ state of either qubit (A or B) of the system a difficult task. Here, we find a means of reducing the 4×4 Hamiltonian matrix of the coupled system to a 2×2 matrix, whereby the mathematics is greatly simplified.

By maintaining a high bias on the control qubit throughout the gate operation, we can force it to remain in its initialized memory state. The 4×4 Hamiltonian matrix of the two-qubit, two-level system can now be reduced to a 2×2

Hamiltonian matrix of a single-qubit system, which is given as

$$H'_B = \Delta_B \sigma_X + (\varepsilon_B \pm \xi)\sigma_Z, \tag{10}$$

which describes the true evolution of qubit B only. The coupling term ξ either adds or subtracts from ε_B depending on whether the expectation value of σ_{ZA} is +1 or −1 in the subspace of target qubit B.

Thus, we have reduced the two-qubit coupled system into an effective single-qubit system involving only the target qubit B. This reduced single-qubit system has two Hamiltonians, as given by Eq. (10), depending upon the state of the control qubit A. The equation for the probability in the $|1\rangle$ state for the target qubit B will be as given by Eq. (5), however, the bias term ε in these equations is now replaced by the "effective" bias term $(\varepsilon_B \pm \xi)$ that can take one of two values depending upon the state of the control qubit A. The effective bias on the target qubit when the control qubit A is in the $|0\rangle$ and $|1\rangle$ states is $(\varepsilon_B + \xi)$ and $(\varepsilon_B - \xi)$, respectively. Therefore, there will now be two frequencies of oscillation for the probability in the $|1\rangle$ state for the target qubit B. Our purpose is to control these frequencies in order to achieve a CNOT gate operation.

IV. CHOICE OF PARAMETERS FOR CNOT GATE

As discussed in the previous section, depending on the state of the control qubit A, there are two oscillation frequencies for the probability of oscillation in the $|1\rangle$ state for the target qubit B, which are given by

$$f_{1,2} = 2\sqrt{[\Delta_B{}^2 + (\varepsilon_B \pm \xi)^2]}, \tag{11}$$

where frequencies f_1 and f_2 correspond to the frequency of the probability oscillation when the control qubit is in the $|0\rangle$ and $|1\rangle$ states, respectively.

From Eq. (5), which shows the probability in the $|1\rangle$ state for a single qubit system, we can see that the term $(\Delta^2 + \varepsilon^2)$ in the denominator of the amplitude term [Eq. (7)] is responsible for the attenuation caused to the amplitude of the oscillations. In this case, since we are dealing with two different effective biases acting on the target qubit B, the effective bias being $(\varepsilon_B + \xi)$ and $(\varepsilon_B - \xi)$, depending on whether the control qubit A is in the $|0\rangle$ and $|1\rangle$ states, respectively, the attenuation to the amplitude is caused by the terms $[\Delta_B{}^2 + (\varepsilon_B + \xi)^2]$ and $[\Delta_B{}^2 + (\varepsilon_B - \xi)^2]$, respectively, in the denominator. In order to achieve a CNOT gate operation, it is required that the target qubit B does not change its state when the control qubit A is in the $|0\rangle$ state. This implies that qubit B, in its transitional state, undergoes an *integer number of complete oscillation cycles*, whereby it returns to its initialized state. Therefore, the attenuation to the amplitude by the term $[\Delta_B{}^2 + (\varepsilon_B + \xi)^2]$ in the denominator, is of no concern as such. When qubit A is in the $|1\rangle$ state, qubit B changes state, i.e., from $|0\rangle$ to $|1\rangle$ and vice versa. This corresponds to *a half cycle oscillation* in addition to an integer number of complete oscillation cycles, i.e., the *target qubit* B *undergoes an odd integer number of half cycles in its transitional state and flips its state*. In this case, we require that there be no attenuation to the amplitude of the oscillations by the term $[\Delta_B{}^2 + (\varepsilon_B - \xi)^2]$ in the denominator. Therefore, with an effective bias of $(\varepsilon_B - \xi)$ acting on the target qubit when the control qubit A is in the $|1\rangle$ state, *it is required that* ε_B *and* ξ *cancel each other in order to realize a switched logic state with no attenuation to the amplitude at a half cycle*. In other words, ξ needs to be equal to ε_B in the transitional state of the target B. The probability function oscillates between 0 and 1 with a frequency of oscillation, $f_2 = 2\Delta_B$, obtained from Eq. (11).

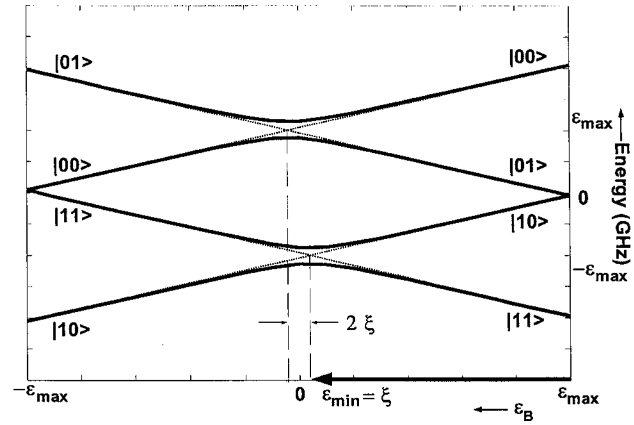

FIG. 1. Energy level diagram of the coupled system of two qubits for the calculated choice of parameters.

From our discussion, it follows that if T is the time step and P and Q are an integer number of complete cycles in the transitional state of target qubit B

$$f_1 = 2\sqrt{[\Delta_B{}^2 + (\varepsilon_B + \xi)^2]} = \frac{P}{T}, \tag{12}$$

and

$$f_2 = 2\sqrt{[\Delta_B{}^2 + (\varepsilon_B - \xi)^2]} = 2\Delta_B = \frac{Q + \frac{1}{2}}{T}. \tag{13}$$

We, thereby, have a system of two equations in two unknowns, which can be exactly solved for. For different values of P, Q, and T, Eqs. (12) and (13) can be used to solve for Δ_B, ξ, and ε_B. The bias on the target qubit B gives the value to which the bias must be pulsed low (ε_{min}) in order to bring the target qubit B to a transitional state, whereby it undergoes oscillations. As mentioned earlier, the target qubit can be brought back to a memory state by pulsing the bias to an "arbitrarily" high value (ε_{max}). There is no upper limit on this value of the bias other than ε_{max} having to be much larger than Δ_B and restrictions imposed by practical considerations.

Figure 1 shows a plot of the four eigenenergies of the coupled system. The bias on the control qubit is maintained at an arbitrarily high value ε_{max}. This splits the system into two separate two-level systems, $|00\rangle$, $|01\rangle$ and $|10\rangle$, $|11\rangle$, centered at $+\varepsilon_{max}$ and $-\varepsilon_{max}$, respectively, depending upon the state of the control qubit A. We start out initially with the target qubit in a memory state ($\varepsilon_B = \varepsilon_{max}$). Suppose the system is initially in the $|11\rangle$ state. The bias on the target qubit B is now clocked low to ε_{min}, which is indicated by means of an arrow in the diagram. This brings the system to the degeneracy point of the $|10\rangle$ and $|11\rangle$ energy levels as the coupling ξ cancels with the bias ε_{min}. The target qubit B undergoes an odd integer number of half-cycle oscillations, as given by Eq. (13), between the $|11\rangle$ and $|10\rangle$ states within the transitional time T and flips its state. At the end of the time step, the bias on the target is pulsed high ($\varepsilon_B=\varepsilon_{max}$), forcing the target qubit once again into a memory state. Similarly, when the system starts out in the $|10\rangle$ state, it evolves to the $|11\rangle$ state.

Suppose the system is initially in the $|00\rangle$ state. When the bias on the target qubit is pulsed low to ε_{min}, the system does not reach the degeneracy point for the $|00\rangle$ and $|01\rangle$ energy levels. The effective bias acting on the target qubit is $2\varepsilon_{min}$ and the qubit undergoes oscillations of reduced amplitude between the $|00\rangle$ and $|01\rangle$ states. Since the qubit undergoes an integer number of complete oscillations within the time step T as given by Eq. (12), it returns to its initialized state. At the end of the time step, the bias on the target is pulsed high ($\varepsilon_B=\varepsilon_{max}$), forcing the target qubit to maintain its memory state. Similarly, when the system starts out in the $|01\rangle$ state, the system evolves back to the $|01\rangle$ state at the end of the time step.

It is important to distinguish between the fixed and controllable parameters in our scheme, which depends on the choice of the quantum system. For instance, if we use superconducting quantum interference devices (SQUIDs) as our choice of a two-level quantum system, the SQUIDs used to implement a CNOT gate using this approach will be fabricated to have the tunneling and coupling parameters fixed to a suitable value calculated as shown in this section. The bias term will be the control parameter, which will be pulsed during experimentation.

We have showed above how parameter values can be calculated for a given choice of time step and the number of complete oscillations. Because of the sensitivity of these parameters, their values are usually fixed. Therefore, instead of starting out with values for the time step (T) and the number of oscillations (P,Q) and then finding the parameter values, the procedure could be reversed, i.e., find T, P, and Q from a given set of Δ_B, ξ, and ε_B.

V. SIMULATION RESULTS—CNOT GATE REALIZATION FOR TWO-QUBIT COUPLED SYSTEM

In the previous section, we reduced the 4×4 Hamiltonian of a two-qubit system into a 2×2 Hamiltonian describing the evolution of the target qubit only under a CNOT gate operation. Using this reduced system, we were able to solve for the parameter values Δ_B, ξ, and ε_B using Eqs. (12) and (13) for different values of T, P, and Q. Since the bias on the control qubit is maintained arbitrarily high throughout (ε_{max}), in order to keep it in its initialized state, the tunneling parameter for qubit A is chosen to be the same as the calculated value for Δ_B.

The parameter values calculated using our reduced system approximation are substituted for in the coupled system Hamiltonian given by Eqs. (2)–(4) for simulation. Figure 2 shows a truth table of the present CNOT operation estimated by the numerical calculation with the detailed values of the probabilities listed in the caption as a matrix.

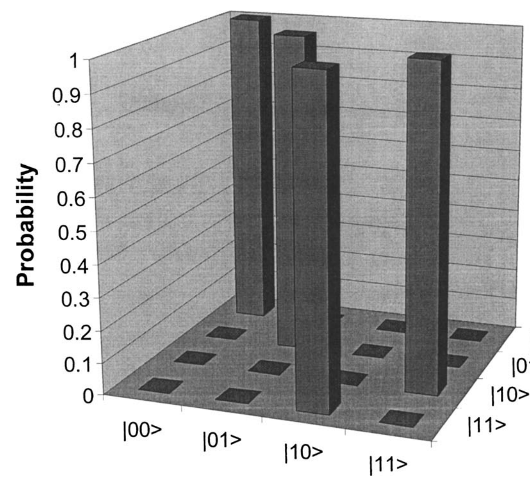

FIG. 2. Truth table of the present CNOT gate operation estimated by the numerical calculation where the values of the probabilities are found to be

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Table I shows the parameter values calculated for a time step T of 10 ns for one-half and one oscillation cycle periods ($P=1,Q=0$) in the transitional state of qubit B. We have chosen 10 ns pulses, as they are experimentally realizable time steps for rf SQUIDs. The simulations were carried out over three time steps where the first and third time steps corresponded to memory states, of 5 ns each, for the target qubit B and the second time step corresponded to a transitional state of 10 ns. Figure 3 shows the bias on the target qubit. The bias on the control qubit A is maintained high throughout. Since the set of equations (12) and (13) are linear, the parameter values for any other time step with the same number of oscillation cycles (same P and Q values) can be obtained by simply multiplying the calculated values by an appropriate factor. For instance, the parameter values for a time step of 1 ns can be obtained by multiplying each of the calculated parameter values, Δ_B, ξ, and ε_B, by a factor of 10.

Figure 4 shows the evolution of probabilities of the computational states of the coupled qubits under a CNOT gate operation. Figures 4(a) and 4(b) show the gate operation when the initial states are $|00\rangle$ and $|01\rangle$, respectively. Qubit B undergoes 1 complete oscillation in its transitional state, whereby it returns to its initial state, $|0\rangle$ or $|1\rangle$. Figures 4(c)

TABLE I. Parameter values for the CNOT gate for $T=10$ ns, $P=1$, and $Q=0$.

Parameter	Value (GHz)
$\Delta_A=\Delta_B$	0.025
ε_{max}	10.0
$\varepsilon_{min}=\xi$	0.022

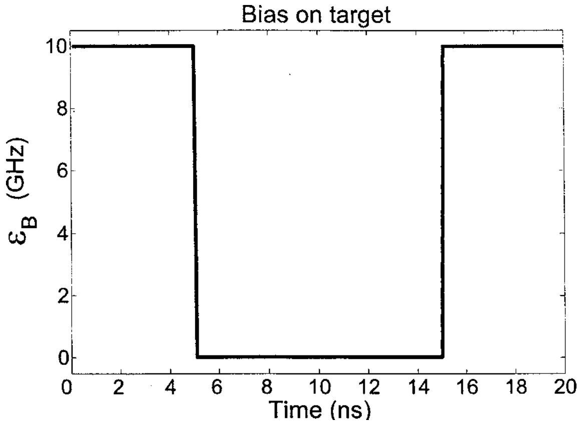

FIG. 3. Bias on the target qubit B. The bias on the control qubit A is maintained high throughout. The first and third time steps of 5 ns each are memory states for the target qubit. The second time step of 10 ns (T) is the transitional state.

and 4(d) show the gate operation when the initial states are $|10\rangle$ and $|11\rangle$, respectively. In this case, the target qubit B undergoes half an oscillation cycle in its transitional state, whereby it switches its state from its initial state $|0\rangle$ to state $|1\rangle$ or from $|1\rangle$ to $|0\rangle$.

Though we have used ideal pulses in our simulations, we find that including rise and fall times in our simulations has little impact on the overall results as long as they are accounted for. We recalculate the pulse width to include the rise and fall times by using the following rule of thumb when $\varepsilon_{max} \gg \xi$

$$T' = T + \left(\frac{\varepsilon_{\max} - 5\Delta}{\varepsilon_{\max}}\right)\left(\frac{(\text{rise time}) + (\text{fall time})}{2}\right), \quad (14)$$

which provides good results for $\varepsilon_{max} \gg \xi$. For a rise time of 4 ns, the new pulse width T' was calculated using Eq. (14) to be 13.95 ns, where we have chosen the rise time equal to the fall time. When the CNOT gate was simulated using these nonideal pulses for the parameter values listed in Table I, the error was found to be less than 1%, which is an improvement over that presented in Ref. [10].

Our previous simulation results only show the operation of the gate as a classical one. In order for the gate to be a quantum gate, its operation needs to be shown for the case when the initial state is a superposition of two states. For example, when the initial state of the system is an equal superposition of the states $|00\rangle$ and $|10\rangle$, the product state $(|0\rangle + |1\rangle)\ |0\rangle$, which has zero degree of entanglement, the system as a whole evolves into the Bell state, a maximally entangled state, as a result of coherence being maintained. Figure 5 shows a plot of the probabilities of the qubits A and B in the $|1\rangle$ state over a total time of 20 ns with half an oscillation ($P=1, Q=0$) in the transitional state of qubit B.

The final state of the system in terms of probability amplitudes in each of the four basis states was found through simulation, using the parameter values listed in Table I, to be

$$|\psi(t)\rangle = 0.7e^{-0.6i}|00\rangle + 0.1e^{-1.6i}|01\rangle + 0.1e^{0.3i}|10\rangle + 0.7e^{-1.6i}|11\rangle \approx \frac{|00\rangle + e^{i\phi}|11\rangle}{\sqrt{2}},$$

where ϕ is the relative phase difference between the two states $|00\rangle$ and $|11\rangle$. The value of the actual calculated probability amplitude shows that the system evolves from the product state into the maximally entangled Bell state. Thus, our technique can be used to put a system into a state of entanglement.

It can also be shown that when the initial state is the EPR state [1], an equal superposition of the $|01\rangle$ and $|10\rangle$ states, the system evolves into the product state $(|0\rangle + |1\rangle)\ |1\rangle$.

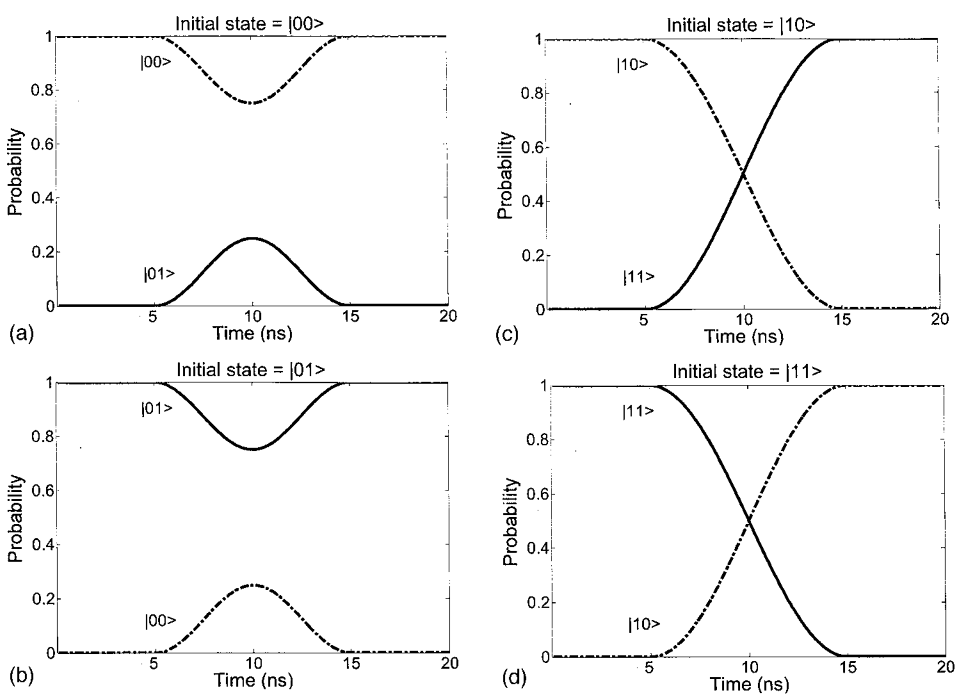

FIG. 4. Evolution of the probabilities of the computational states of the two-qubit coupled system under a CNOT gate operation for each of the four initial states. The total time is 20 ns with a transitional state T of 10 ns.

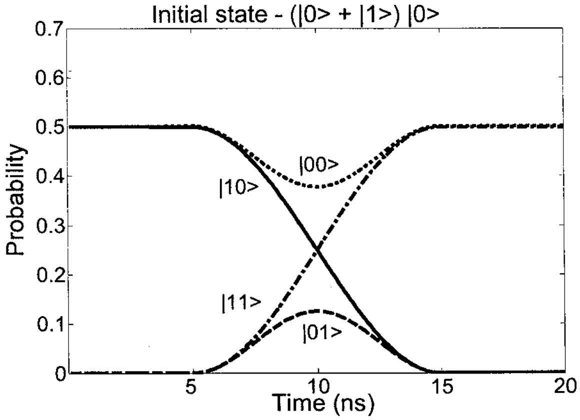

FIG. 5. Realization of CNOT gate operation for a superposition of states corresponding to one-half or one oscillation cycles ($P=1,Q=0$) in the transitional state of qubit B. The time step, for the transitional state is $T=10$ ns and the total time is 20 ns. The system is initially in a product state, an equal superposition of the $|00\rangle$ and $|10\rangle$ states. The final state of the system is the Bell state, a maximally entangled state.

VI. CNOT GATE OPERATION USING A MULTILEVEL TWO-SQUID COUPLED SYSTEM

To demonstrate the feasibility of the pulsed bias scheme proposed above in multilevel coupled qubits, we apply it to a system of two coupled rf SQUID qubits with realistic device parameters. A rf SQUID consists of a superconducting loop of inductance L interrupted by a Josephson tunnel junction. The tunnel junction is characterized by its critical current I_c, shunt capacitance C, and shunt resistance R. A flux-biased SQUID with total magnetic flux Φ enclosed in the loop is analogous to a "flux" particle of mass $m=C\Phi_0^{\,2}$ moving in a one-dimensional potential, where $\Phi_0=h/2e$ is the flux quantum. The Hamiltonian of a rf SQUID can be written as [6]

$$H(x)=\frac{p^2}{2m}+U(x), \tag{15}$$

where $x=\Phi/\Phi_0$ is the canonical coordinate of the "flux" particle, $p=-i\partial/\partial x$ is the canonical momentum conjugate to x, and $U(x)$ is the potential energy given by

$$U(x)=\frac{m\omega_{LC}^{\;2}(x-x_e)^2}{2}-E_J\cos(2\pi x). \tag{16}$$

Here, $E_{\mathrm{J}}=I_{\mathrm{c}}\Phi_0/2\pi=m\omega_{\mathrm{LC}}^{\;2}\beta_{\mathrm{L}}/4\pi^2$ is the Josephson coupling energy, $\omega_{\mathrm{LC}}=(LC)^{-1/2}$ is the characteristic frequency of the SQUID, $\beta_{\mathrm{L}}=2\pi LI_{\mathrm{c}}/\Phi_0$ is the potential shape parameter, and $x_e=\Phi_{\mathrm{e}}/\Phi_0$ is the normalized external flux bias.

The coupled SQUID qubits system consists of two single rf SQUID qubits, a control qubit and a target qubit, coupled inductively by the mutual inductance M. For simplicity, we assume that the two SQUIDs are identical ($C_1=C_2=C$, $L_1=L_2=L$, and $R_1=R_2=R$). We also assume that the external magnetic fluxes applied to the two SQUIDs are $\Phi_{\mathrm{e}1}$ and $\Phi_{\mathrm{e}2}$, and the total fluxes are Φ_1 and Φ_2, respectively. The Hamiltonian of the coupled SQUID flux qubits is given by [21]:

$$H(x_1,x_2)=H_0(x_1)+H_0(x_2)+H_{12}(x_1,x_2), \tag{17}$$

where $H_0(x_i)$ is Hamiltonian of the ith single qubit given by Eq. (15) and H_{12} is the interaction between the two SQUID qubits and is given by

$$H_{12}(x_1,x_2)=m\omega_{LC}^{\;2}k(x-x_{e1})(x-x_{e2}). \tag{18}$$

Here, $x_{ei}=\Phi_{\mathrm{ei}}/\Phi_0$ is the normalized external flux bias of the ith qubit and $k=M/L$ is the coupling coefficient. The coupled SQUID qubits are a multilevel system. The eigenenergies E_n and eigenstates $|n)$ of the coupled qubits are computed by solving the Schrödinger equation with $H(x_1,x_2)$ using the two-dimensional Fourier-grid Hamiltonian method [22] using 20 eigenstates. For weak coupling, the eigenstate of the coupled qubits $|n)$ can be well approximated by the product of an eigenstate of the control qubit $|i\rangle$ and that of the target qubit $|j\rangle, |n)=|ij\rangle=|i\rangle|j\rangle$. If both x_{e1} and x_{e2} are around 0.5, the coupled SQUID qubits have four wells in the potential energy surface [21]. The four computational states are chosen to be the lowest eigenstates of each well and are denoted by $|1)=|10\rangle$, $|2)=|11\rangle$, $|3)=|00\rangle$, and $|4)=|01\rangle$. At the avoided crossing points, the spacing between the product states are $0.538\,34/\omega_{\mathrm{LC}}=42.840$ GHz ($|10\rangle\pm|11\rangle$) and $0.538\,30/\omega_{\mathrm{LC}}=42.837$ GHz ($|00\rangle\pm|01\rangle$), respectively, which are very close due to weak coupling. The values of x_{e2} at the avoided crossing points are 0.499 933 3 and 0.500 061 7, respectively. The device parameters for the SQUIDs are $Z_0=50\ \Omega$ (i.e., $L=100$ pH and $C=40$ fF), $\beta_{\mathrm{L}}=1.15$, and $\omega_{\mathrm{LC}}=5\times10^{11}$ rad/s.

To implement two-qubit gates with the coupled SQUID flux qubits, we apply a dc pulse to the target qubit. The interaction between the pulse and the coupled qubits is given by

$$V(x_1,x_2,t)=m\omega_{LC}^{\;2}\left[(x_2-x_{e2})x_\varepsilon(t)+\frac{x_\varepsilon(t)^2}{2}+\frac{k(x_1-x_{e1})x_\varepsilon(t)}{2}\right], \tag{19}$$

where $x_\varepsilon(t)$ is the magnetic flux (normalized to Φ_0) coupled to the target qubit from the dc pulse. According to the pulsed bias scheme, the peak flux of the dc pulse $x_{\varepsilon0}$ is chosen to bring the system from its initial eigenstate to one of the product states. To realize the CNOT gate, a dc pulse with peak flux $x_{\varepsilon0}=-0.4333$ was applied to the target qubit to bring the system to the avoided crossing point at which $x_{e2}=0.499\,933\,3$. The configuration of the SQUID is at $x_{e1}=0.499$, $x_{e2}=0.4995$, and $k=0.0005$.

Figures 6(a)–6(d) show a plot of the evolution of the probabilities of the computational states for the coupled SQUID qubits starting in each of the four initial states $|10\rangle$, $|11\rangle$, $|00\rangle$, and $|01\rangle$, respectively. The parameter values were chosen so as to realize one-half and two oscillations in the transitional states ($P=2$ and $Q=0$). Figures 6(a) and 6(b) show the evolution from the initial state $|10\rangle$ to the final state $|11\rangle$ and from the initial state $|11\rangle$ to the final state $|10\rangle$. Figures 6(c) and 6(d) show the evolution when the system starts out initially in the $|00\rangle$ and $|01\rangle$ states, respectively. From these plots, we can see that although the probabilities

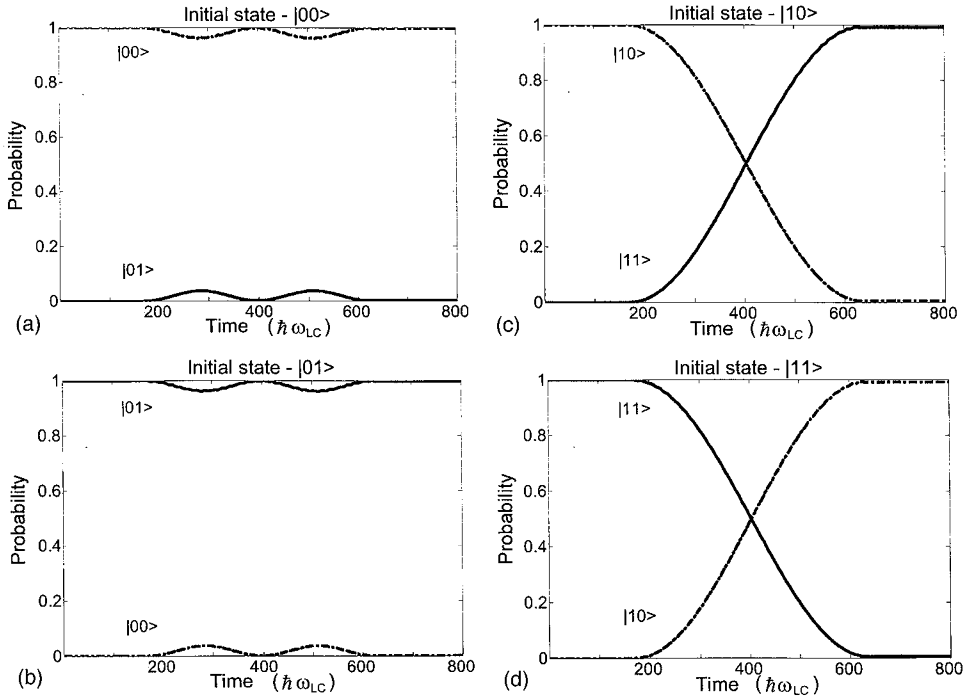

FIG. 6. Evolution of probabilities of the computational states for the coupled SQUID qubits for the initial states (a) $|00\rangle$, (b) $|01\rangle$, (c) $|10\rangle$, and (d) $|11\rangle$, respectively.

of the states $|00\rangle$ and $|01\rangle$ are not always zero for the duration of the pulse, the coupled qubits return back to the initial states after the pulse. The maximum probabilities of these states will tend to zero with an increase in the distance between the two avoided crossing points in x_{e2}, which can be accomplished by increasing the coupling. Thus, by applying the dc pulse to the target qubit of the coupled SQUID flux qubits system, the CNOT gate is realized successfully.

VII. TOFFOLI GATE

The controlled-controlled NOT (CCNOT) gate, or the Toffoli gate, uses three qubits. Like the CNOT, it is a reversible and universal gate. There are three inputs to the gate, two of which, A and B, are control qubits and the third, C, is the target. The target qubit flips its state only when both the control qubits are in the logic $|1\rangle$ state.

Methods have been proposed for realizing the Toffoli gate using two-bit CNOT gates and some one-bit gates [4]. In this section, we will show how this gate can be implemented using the reduced Hamiltonian approach discussed in Sec. IV.

Consider a system of three qubits, A, B, and C, where A and B are control qubits and C is a target qubit coupled to A and B. The two control qubits A and B are not coupled to each other. The target qubit C is coupled to each of the controls through the coupling terms ξ_{AC} and ξ_{BC}, respectively (see Fig. 7).

The Hamiltonian of the system is given as

$$H = H_A + H_B + H_C + H_{AC} + H_{BC}, \tag{20}$$

where

$$H_{AC} = \xi_{AC}\sigma_{ZA}\sigma_{ZC}, \tag{21}$$

and

$$H_{BC} = \xi_{BC}\sigma_{ZB}\sigma_{ZC}. \tag{22}$$

Here, H_A, H_B, and H_C are the uncoupled Hamiltonians for qubits A, B, and C, respectively. H_{AC} is the interaction energy for the two qubits A and C; H_{BC} is the interaction energy for the two qubits B and C; ε_A, ε_B, and ε_C are the biases; Δ_A, Δ_B, and Δ_C are half the uncoupled tunneling frequencies of A, B, and C, respectively; ξ_{AC} is the coupling factor between qubits A and C; ξ_{BC} is the coupling factor between qubits B and C; and σ_{XA}, σ_{ZA}, σ_{XB}, σ_{ZB}, σ_{XC}, and σ_{ZC} are the outer products of the Pauli matrices with identity matrices.

By keeping ε_A and ε_B large, control qubits A and B are maintained in memory states. Using the paradigm of Sec. IV, in this case for a three-qubit system, the 8×8 Hamiltonian matrix of the system can be reduced to a 2×2 Hamiltonian matrix, for qubit C, of the form

$$H'_C = \Delta_C\sigma_X + (\varepsilon_C \pm \xi_{AC} \pm \xi_{BC})\sigma_Z, \tag{23}$$

where the coupling term, ξ_{AC} (ξ_{BC}) either adds or subtracts from ε_C depending on whether the expectation value of σ_{ZA} (σ_{ZB}) is $+1$ or -1 in the subspace of target qubit C. The expectation value of σ_{ZA} (σ_{ZB}) is $+1$ when the state of control qubit A (B) is $|0\rangle$ and the value of σ_{ZA} (σ_{ZB}) is -1 when the state of control qubit A (B) is $|1\rangle$.

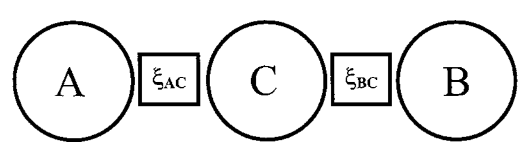

FIG. 7. A three-qubit, two-level coupled system. A and B are the control qubits and C is the target qubit. The target is coupled to each of the two control qubits through the coupling terms ξ_{AC} and ξ_{BC}. The two control qubits are not coupled to each other.

The probability of the target qubit C in the $|1\rangle$ state is as given by Eqs. (5)–(8), where the bias term ε in these equations is now replaced by the "effective" bias term $(\varepsilon_C \pm \xi_{AC} \pm \xi_{BC})$ depending upon the states of the control qubits A and B. Therefore, there are four different frequencies as follows

$$f = 2\sqrt{[\Delta_C{}^2 + (\varepsilon_C \pm \xi_{AC} \pm \xi_{BC})^2]}. \quad (24)$$

Here, if we choose ξ_{AC} and ξ_{BC} to be equal to each other, due to symmetry, we will have only three frequencies given by

$$f_1 = 2\sqrt{[\Delta_C{}^2 + (\varepsilon_C + 2\xi_{AC})^2]}, \quad (25)$$

$$f_2 = 2\sqrt{[\Delta_C{}^2 + (\varepsilon_C - 2\xi_{AC})^2]}, \quad (26)$$

$$f_3 = 2\sqrt{(\Delta_C{}^2 + \varepsilon_C{}^2)}. \quad (27)$$

For the operation of the CCNOT gate, we require that the target qubit, C, flip its state only when each of the control qubits, A and B, are in the $|1\rangle$ state, which corresponds to an odd integer number of half-cycle oscillations. In order to avoid any attenuation at a half cycle, we need ε_C to cancel with the coupling term, $2\xi_{AC}$, and therefore,

$$\xi_{AC} = \xi_{BC} = \frac{\varepsilon_C}{2}. \quad (28)$$

From Eqs. (26) and (28), we have

$$f_2 = 2\Delta_C = \frac{m/2}{T}, \quad (29)$$

where m is an odd integer ($m/2$ is an odd integer number of half cycles) and T is the total time step.

Equation (25) corresponds to the state when both the control qubits, A and B, are in the $|0\rangle$ state and the target qubit, C, is in either state $|0\rangle$ or $|1\rangle$. For the target qubit C to maintain its initialized state, it is required that it undergo an integer number of complete oscillation cycles in its transitional state, when ε_C is clocked low. From Eq. (29), we know that frequency f_2 corresponds to an odd integer number of half cycles. *For frequency f_1 to realize a complete number of oscillation cycles, it needs to be an even integer multiple of f_2*. In other words, we have from Eqs. (25), (28), and (29),

$$f_1 = 2\sqrt{[\Delta_C{}^2 + (2\varepsilon_C)^2]} = (2P)f_2 = (2P)(2\Delta_C), \quad (30)$$

where P is an integer.

Similarly, Eq. (27) corresponds to each of the four states $|010\rangle$, $|011\rangle$, $|100\rangle$, and $|101\rangle$, where one of the two control qubits is in the $|1\rangle$ state and the other is in the $|0\rangle$ state. In each case, the target qubit C needs to undergo an integer number of complete oscillation cycles. In other words, *frequency f_3 needs to be an even integer multiple of f_2*. Hence, we have from Eqs. (27)–(29),

$$f_3 = 2\sqrt{(\Delta_C{}^2 + \varepsilon_C{}^2)} = (2Q)f_2 = (2Q)(2\Delta_C), \quad (31)$$

where Q is an integer.

To solve for the parameter values Δ_C and ε_C, we choose ε_C, ξ_{AC}, and ξ_{BC} in accordance with Eq. (28) to be functions of Δ_C

$$\varepsilon_C = 2\xi_{AC} = 2\xi_{BC} = \frac{\sqrt{M}}{2}\Delta_C, \quad (32)$$

where M is an integer. Using Eq. (32) in Eqs. (30) and (31), we have

$$\sqrt{(\Delta_C{}^2 + M\Delta_C{}^2)} = P(2\Delta_C),$$

$$\sqrt{\left(\Delta_C{}^2 + \frac{M}{4}\Delta_C{}^2\right)} = Q(2\Delta_C). \quad (33)$$

The set of equations (29) and (33) are solved for Δ_C, P, and Q for different values of m, T, and M. In our simulations, we used a time step T of 10 ns. We chose the value of m to be 5, which gave $2\frac{1}{2}$ oscillations whenever the target qubit C, in its transitional state, underwent a reversal of state. From Eq. (29), the value of Δ_C can be directly calculated. For our choice of T and m, Δ_C was calculated to be 0.125 GHz.

Next, for different integer values of M, the set of equations (33) were evaluated to solve for P and Q. With M being an integer, it was not possible to obtain exact integer values for both P and Q simultaneously, i.e., either one of them evaluated to be an integer while the other was a number close to an integer. For instance, for $M=60$, P and Q evaluated to be 3.9 ($\sim$4.0) and 2.0, respectively, while for $M=63$, P and Q evaluated to be 4.0 and 2.05 ($\sim$2.0), respectively. This is the case even when both the coupling terms are not equal. For our simulations, we chose the value of M to be 60 from which, using Eq. (32), the values of ε_C, ξ_{AC}, and ξ_{BC} were calculated to be 0.484 GHz, 0.242 GHz, and 0.242 GHz, respectively. This means that for each of the states $|000\rangle$ and $|001\rangle$, the target C undergoes 20 oscillation cycles in its transitional state, whereby it returns to its initialized state. In each of the states $|010\rangle$, $|011\rangle$, $|100\rangle$, and $|101\rangle$, qubit C undergoes ten complete oscillations in its transitional state to return to its initialized state. From Eq. (29) and the evaluated value of Δ_C, the qubit undergoes $2\frac{1}{2}$ oscillation cycles in its transitional state in each of the states $|110\rangle$ and $|111\rangle$ and, hence, flips its state.

VIII. SIMULATION RESULTS OF TOFFOLI GATE

Like the CNOT gate, the simulations for the Toffoli gate were carried out over a total time span of 20 ns where the first and third time steps of 5 ns each were memory states and the second time step of 10 ns was a transitional state. The biases on the two control qubits were maintained high throughout while the bias on the target qubit was pulsed similar to that shown in Fig. 3 (the high and low values being listed in Table II). Depending upon the state of the control qubits, target C either flipped its state (when both controls were in the $|1\rangle$ state) by undergoing $2\frac{1}{2}$ oscillations or returned to the state it was in at the start of the time step by undergoing an integer number of complete oscillations.

TABLE II. Parameter values for the Toffoli gate. The values were calculated as discussed in Sec. VII. The time step T in the transitional state is 10 ns and the total time is 20 ns. The values of m, M, P, and Q were chosen to be 5, 60, 3.9, and 2, respectively.

Parameter	Value (GHz)
$\Delta_A=\Delta_B=\Delta_C$	0.125
$\xi_{AC}=\xi_{BC}$	0.242
ε_{max}	10.0
ε_{min}	0.484

Table II lists the corresponding parameter values for the Toffoli gate operation. The values of Δ_A and Δ_B were made equal to the calculated value of Δ_C. Figure 8 shows the truth table of the Toffoli gate estimated by the numerical calculation. From the simulation results, it is clear that the CCNOT gate was realized using our approach.

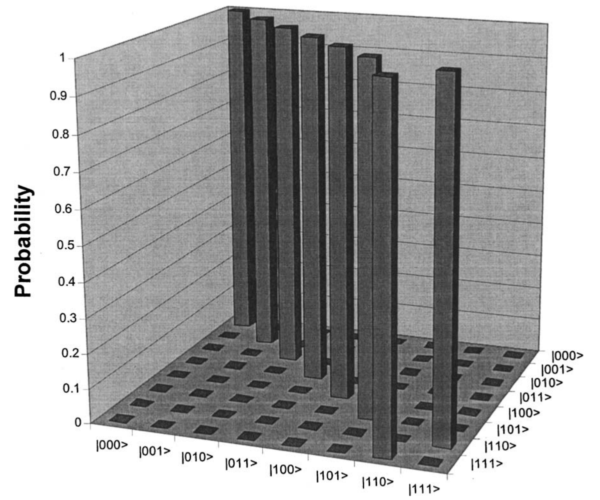

FIG. 8. Truth table of the present Toffoli gate operation estimated by the numerical calculation.

IX. CONCLUSION

We have shown in this paper how to realize quantum gates by pulsing the bias of a quantum two-level system. We have shown how to realize a CNOT gate using a two-qubit, two-level coupled system. Under a CNOT gate operation, by keeping the state of control qubit A constant, we reduced the 4×4 Hamiltonian to a 2×2 Hamiltonian for the target qubit B. Using the reduced Hamiltonian, we were able to solve for parameter values for the coupling term, tunneling frequency, and bias in the transitional state. Since the governing equations used to calculate the parameter values are linear, the parameter values are resizable, depending upon the pulse width; therefore, there is no theoretical restriction on the range of calculated values for the parameters. We further demonstrated our proposed scheme by simulating the CNOT gate operation for a multilevel system of two coupled SQUIDs using the parameters calculated.

We have also shown how the same approach can be used to realize the Toffoli gate. In this case, the state of the two control qubits are kept constant and the 8×8 Hamiltonian of the three-qubit system is reduced to a 2×2 Hamiltonian for target C. The parameter values for proper gate operation were calculated using this approach and a CCNOT gate was realized in simulation.

ACKNOWLEDGMENTS

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