

# Adiabatic quantum optimization with qudits

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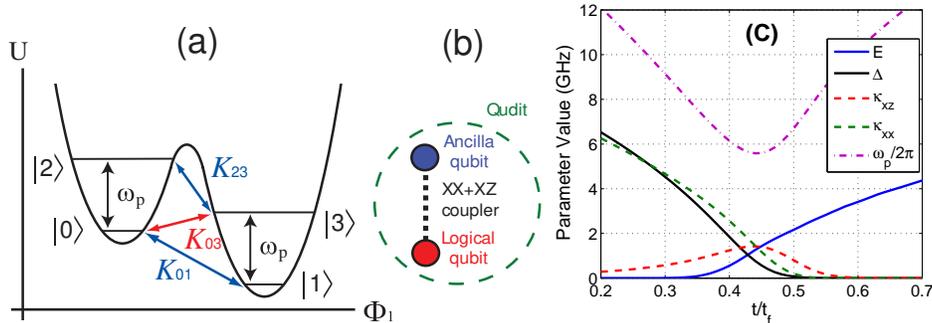
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**Abstract.** Most realistic solid state devices considered as qubits are not true two-state systems but multi-level systems. They can approximately be considered as qubits only if the energy separation of the upper energy levels from the lowest two is very large. If this condition is not met, the upper states may affect the evolution and therefore cannot be neglected. Here, we consider devices with double-well potential as basic logical elements, and study the effect of higher energy levels, beyond the lowest two, on adiabatic quantum optimization. We show that the extra levels can be modeled by adding additional (ancilla) qubits coupled to the original (logical) qubits. The presence of these levels is shown to have no effect on the final ground state. We also study their influence on the minimum gap for a set of 8-qubit spin glass instances.

## 1 Introduction

Quantum information processing has been one of the fastest growing interdisciplinary research areas over the past decade, with the promise of revolutionizing the concept and possibilities of future computation [1]. Unlike classical information processing in which information is stored as classical states of the classical bits, in quantum information processing, information is stored as quantum states of qubits which are two-state quantum systems representing the basic logical elements of quantum information. Most realistic devices, however, are not ideal two-state systems. Therefore, the ideal two-state (qubit) model, commonly used in quantum information, is only an approximation to their true quantum behavior. For example, all superconducting qubits, whether charge [2], hybrid [3], phase [4], or flux [5–8] qubits, have several energy levels, only lowest two considered as the relevant qubit states.

Flux qubits generally have potential energy (in the flux basis) in the form of a double-well potential similar to the one illustrated in Fig. 1a [5–8]. In the limit of infinite barrier height between the two wells, one can treat each well separately and obtain two sets of quantized energy levels localized within the wells. At finite barrier height, these localized states are not true eigenstates of the Hamiltonian anymore and therefore are



**Fig. 1.** (a) Schematic diagram of a double-well potential with the first four metastable energy levels and the tunneling amplitudes ( $K_{ij}$ ) between them. (b) A four-state model of the system represented by two coupled qubits. (c) Parameters of the qudit Hamiltonian (3) during an annealing process, calculated for an rf-SQUID with experimentally motivated parameters (see the appendix). All energy scales are divided by  $\hbar$  (Planck constant) and converted into GHz.

metastable, which means a system initialized in one of them will eventually transition out of it via a tunneling process. The true eigenstates of the Hamiltonian are indeed coherent mixtures or superpositions of those localized states. One may still represent the system in the basis of those localized states by introducing off-diagonal elements of the Hamiltonian which provide tunneling amplitudes between them.

It is assumed that when the two lowest energy states dominate the dynamics of the system at low temperatures and small energy bias, one can consider this two-state system as a qubit. However, if the energy bias is comparable to the energy separations within each well,  $\omega_p$ , or the temperature is large enough to allow occupation of higher energy levels, then the two-state model does not describe correctly the quantum behavior of the device. In these situations, one must include the occupied energy levels in the description of the quantum system being studied. Systems with  $d > 2$  energy levels are commonly referred to as qudits.

One of the important paradigms of quantum information processing is adiabatic quantum computation (AQC) [9] which is known to be a universal model of quantum computation [10, 11]. In AQC, the Hamiltonian of the system, generally written as  $H_S(t) = \Delta(t)\mathcal{H}_B + E(t)\mathcal{H}_P$ , slowly evolves as  $\Delta(t)$  decreases and  $E(t)$  increases monotonically with time  $t$ . At the beginning of the evolution,  $E(0) \approx 0$  and the Hamiltonian is dominated by the dimensionless Hamiltonian  $\mathcal{H}_B$ , with a ground state that is usually a superposition of all states in the computation basis. At

the end of the evolution,  $\Delta(t_f) \approx 0$  and the Hamiltonian is dominated by the (dimensionless) problem Hamiltonian  $\mathcal{H}_P$ . If the evolution is slow enough, the final state of the system will represent the ground state of  $\mathcal{H}_P$  with high fidelity, which is designed to solve the intended problem. The time-dependent energy scales  $\Delta(t)$  and  $E(t)$  are usually not independent and both are controlled by one external parameter. A typical example of these functions based on a superconducting realization of the hardware [12] is provided in Fig. 1.

In this article, we focus on a special version of AQC known as adiabatic quantum optimization (AQO). In AQO,  $\mathcal{H}_P$  is diagonal in the logical basis, therefore the final ground state is a classical state that minimizes the energy, hence can be considered as an optimized solution to a cost function. In the literature, AQO is sometimes called quantum annealing [13, 14], as it uses quantum fluctuations for annealing in a similar way as thermal fluctuations are used in classical annealing. We are mainly interested in the transverse Ising Hamiltonian:

$$\mathcal{H}_B = -\frac{1}{2} \sum_{i=1}^N \sigma_x^{(i)}, \quad \mathcal{H}_P = \sum_{i=1}^N h_i \sigma_z^{(i)} + \sum_{i,j=1}^N J_{ij} \sigma_z^{(i)} \sigma_z^{(j)}. \quad (1)$$

where,  $\sigma_{x,z}^{(i)}$  are Pauli matrices corresponding to the  $i$ th qubit, and  $h_i$  and  $J_{ij}$  are dimensionless energy biases and coupling coefficients respectively. An interesting and important question is, how would an adiabatic quantum optimizer perform using realistic multi-level devices (qudits) instead of idealized qubits.

The paper is organized in the following way. In Sec. 2, we consider a quantum device with a double-well potential, such as a superconducting flux qubit, as a physical implementation of a qubit. We describe such a system by an effective tunneling Hamiltonian with finite number of levels and represent that with a few coupled qubits. We derive the parameters of the coupled qubit Hamiltonian representing the qudit in terms of the original tunneling Hamiltonian. In Sec. 3 we discuss how AQO is possible with such multi-qudit system. We study the effect of the extra energy levels on the minimum gap. Section 4 summarizes our findings and provides conclusions to our results.

In the main body of this paper we treat the single logical element of quantum information as a double-well potential illustrated in Fig. 1. The main discussion of the paper is independent of the physical structure behind the double-well potential. We provide a detailed discussion of an example, i.e., rf-SQUID, in the appendix. We use such an rf-SQUID

Hamiltonian with realistic parameters to find the parameters of the qudit Hamiltonian used in our numerical simulations. All parameters are extracted from experimental implementation, therefore the numerical results we provide here are expected to closely represent the physical reality.

## 2 Single qudit Hamiltonian

Let us consider a system with a double-well potential similar to the one depicted in Fig. 1a. As we discussed before, we would like to write the Hamiltonian of this system in the basis of states that are localized within the wells. Such states are not true eigenfunctions of the Hamiltonian and therefore are metastable towards tunneling to the opposite well. Therefore, the resulting Hamiltonian in this basis will have off-diagonal terms corresponding to transitions between states in opposite wells. However, there are no off-diagonal terms corresponding to transitions within a single well, as we require states within a well to be stationary. Intra-well transitions are induced only by environmental relaxation.

Let  $|l\rangle$  denote localized states within the wells. We use even (odd) state numbers, i.e.,  $l = 2n$  ( $2n+1$ ), with  $n = 0, 1, 2, \dots$ , to denote states that are localized in the left (right) well (see Fig. 1a). For the lowest  $M$  energy levels ( $M$  is taken to be even), the effective  $M \times M$  tunneling Hamiltonian is written as

$$H_S = \sum_{l=0}^{M-1} E_l |l\rangle\langle l| + \sum_{n,m=0}^{M/2-1} K_{2n,2m+1} (|2n\rangle\langle 2m+1| + |2m+1\rangle\langle 2n|) \quad (2)$$

where  $E_l$  is the energy expectation value for state  $|l\rangle$  and  $K_{2n,2m+1}$  is the tunneling amplitude between states  $|2n\rangle$  and  $|2m+1\rangle$ , which exist in the opposite wells. Notice that there is no matrix element between states on the same well:  $\langle 2n|H_S|2m\rangle = \langle 2n+1|H_S|2m+1\rangle = 0$ , which means that the states are metastable only towards tunneling to the other side, or the states are quasi-eigenstates of the Hamiltonian within their own sides. In the appendix, we explain how to arrive at such an effective tunneling Hamiltonian for a bistable rf-SQUID and how to extract the parameters of such Hamiltonian from the original rf-SQUID Hamiltonian.

Reading out the state of the device is usually done by identifying left and right wells, hence logical “0” and “1” states. For example, in a flux qubit the two directions of the flux generated by the persistent current in the superconducting loop identify the two wells of the potential, hence the logical “0” and “1” states. One therefore measures the magnetic flux

at the end of the evolution to detect the logical state of the system. Since all energy levels in the left (right) well yield a negative (positive) flux, we associate all of them with logical “0” (“1”). Therefore, all the levels within one well are *logically equivalent*. In other words, the quantum numbers distinguishing states within a well are logically irrelevant. Those degrees of freedom, however, may participate in the dynamics and have to be taken into account in the quantum dynamics when studying the performance of such a system.

In principle, there could be a large number of energy levels in the full spectrum of the double-well potential, not all of them relevant for the dynamics. Let us assume that there are a total of  $M = 2^m$  relevant states that participate in the dynamics. We can denote state  $|l\rangle$  by  $|x_{m-1}\dots x_2x_0\rangle$ , with  $x_i \in \{0,1\}$ , where  $l = \sum_{i=0}^{m-1} 2^i x_i$ , hence the string  $x_{m-1}\dots x_2x_0$  is the binary representation of  $l$ . With the above even-odd representation of states, all states on the left well correspond to  $x_0 = 0$  (even binary numbers), and all states on the right well correspond to  $x_0 = 1$  (odd binary numbers). Now assume that each variable  $x_i$  represents the state of one qubit. Thus, we have an effective system of  $m$  qubits representing the qudit. Only one of the qubits, i.e., the one representing  $x_0$ , determines the logical state of the system. We therefore call that qubit “logical”, and the other  $m-1$  ones “ancilla” qubits.

For simplicity we focus only on  $M = 4$  levels (i.e.,  $m = 2$  qubits representing a qudit). We denote the left states as  $|00\rangle$  and  $|10\rangle$  and the right states as  $|01\rangle$  and  $|11\rangle$ . These four states can be represented by two coupled qubits, as shown in Fig. 1b, the bottom (top) one is taken to be the logical (ancilla) qubit. In order to distinguish between logical and ancilla qubits in the Hamiltonian, we label the Pauli matrices associated with the logical qubit by  $\sigma_\alpha$  and those associated with the ancilla qubit by  $\tau_\alpha$ , where  $\alpha = x, z$ . We use the convention  $\sigma_z|0\rangle = -|0\rangle$ , and  $\sigma_z|1\rangle = |1\rangle$ , and similarly for  $\tau_z$ . The effective two qubit Hamiltonian can therefore be written as

$$H_{eff} = -\frac{1}{2}(\epsilon\sigma_z + \Delta\sigma_x) + \frac{1}{2}[\omega_p\tau_z + \kappa_{xz}\sigma_x(1 + \tau_z) + \kappa_{xx}\sigma_x\tau_x]. \quad (3)$$

State  $|0\rangle$  of the ancilla qubit corresponds to the two lowest energy states in the two wells and the  $|1\rangle$  of the ancilla qubit provides the two upper energy levels, which are separated from the lower ones by an energy difference equal to the plasma frequency  $\omega_p$  ( $\hbar = 1$ ). It is easy to show that (3) is equivalent, up to a constant energy, to Hamiltonian (2), with  $M = 4$ , if

$$\epsilon = E_0 - E_1 = E_2 - E_3, \quad \omega_p = E_2 - E_0 = E_3 - E_1, \quad (4)$$

$$\Delta = -2K_{01}, \quad \kappa_{xz} = K_{23} - K_{01} \approx K_{23}, \quad \kappa_{xx} = 2K_{03} = 2K_{12}. \quad (5)$$

As can be seen, the coupling between logical and ancilla qubits are of XX+XZ type. Figure 1c illustrates typical values of these parameters during an annealing process based on the experimentally realized 8-qubit processor described in Ref. [12] (see the appendix).

### 3 Adiabatic quantum optimization with qudits

We now generalize the above formulation for a single qudit to a coupled multi-qudit system. The coupling is usually via the dominant degree of freedom, which for flux qubits is the magnetic flux. In the multi-qubit representation of a qudit discussed in the last section, the state of the logical qubits represent the direction of the flux degree of freedom. Therefore the coupling should be via the logical qubits, leading to a ZZ coupling term in the Hamiltonian. In practice, the magnetic flux generated by the flux qubit is different if the qubits is in its excited state within a well. As a result, the effect of the ancilla qubit states on the overall qubit coupling is small, and thus is neglected in our formulation.

Given a graph of coupled qubits, in order to recast the problem in the form of coupled qudits, it is enough to connect to each qubit in the original problem an ancilla qubit via an XX+XZ coupling. Ancilla qubits are coupled only to their corresponding logical qubits; there is no coupling between the logical and ancilla qubits of other qudits. Figure 2 illustrates such a situation for an example graph of four coupled qubits.

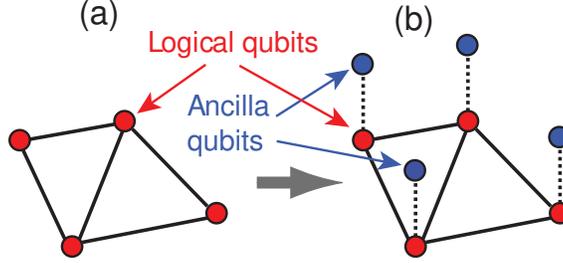
In the case of  $N$  qubits, the corresponding Hamiltonian is

$$H_S = \Delta(t)\mathcal{H}_B + E(t)\mathcal{H}_P \quad (6)$$

$$+ \frac{1}{2} \sum_{i=1}^N \left[ \omega_p^{(i)}(t)\tau_z^{(i)} + \kappa_{xz}^{(i)}(t)\sigma_x^{(i)}(1 + \tau_z^{(i)}) + \kappa_{xx}^{(i)}(t)\sigma_x^{(i)}\tau_x^{(i)} \right].$$

where  $\mathcal{H}_B$  and  $\mathcal{H}_P$  are dimensionless Hamiltonians defined by (1). The first line is identical to the ordinary multi-qubit transverse Ising Hamiltonian and the second line is the contribution of the ancilla qubits.

Figure 1c shows the result of calculation of parameters of Hamiltonian (3) as a function of time during the annealing process, using an rf-SQUID model with experimentally motivated parameters as explained in the appendix. As expected  $\Delta(t)$  decreases and  $E(t)$  increases monotonically with time as required. Notice the non-monotonic variation of  $\omega_p$ , which represents the energy separation of the upper energy levels from the lowest two (see Fig. 1a). To be able to approximate a qudit by a



**Fig. 2.** (a) An example of a multi-qubit graph consisting of 4 qubits (circles) and 5 ZZ couplers (solid lines). (b) The same graph made of 4 qudits, each being a four-state system represented by a logical (bottom) and an ancilla (top) qubit, coupled to each other via a  $XX+XZ$  coupler (dashed lines).

two-state qubit, it is necessary that the excited states within each well be far above the lowest energy levels. This puts a limit on the parameter of the problem Hamiltonian:  $h_i, J_{ij} \ll \omega_p/E(t)$ . If this condition is not met, the energy bias of the qubits can become so large that the lowest state in one well becomes close to the excited state in the next well (see Fig. 1a as an example), hence the two-state model for the device fails to hold. The important question is: Can we still solve the intended optimization problems using such devices? As we shall see the answer is yes.

At the end of the evolution, the barrier between the two wells becomes so large that all tunnelings between the lowest energy levels will stop. This means that all the off-diagonal elements of the Hamiltonian will vanish:  $\Delta = \kappa_{xx}^{(i)} = \kappa_{xz}^{(i)} = 0$ . It is easy to see that in the absence of these off-diagonal elements, the logical and ancilla qubits decouple from each other and the ground state of the total Hamiltonian (6) will be the ground state of the original Ising Hamiltonian  $\mathcal{H}_P$  for the logical qubits with all the ancilla qubits being in state  $|0\rangle$ . Therefore, for the purpose of optimization, the ancilla qubits have no effect on the final ground state even if  $h_i, J_{ij} > \omega_p/E(t)$ . They, however, affect the dynamics of the system as we shall see. This means that *AQO can be performed using qudits instead of qubits regardless of the final Hamiltonian*. The effect of the upper energy levels on the computation time is yet to be discussed.

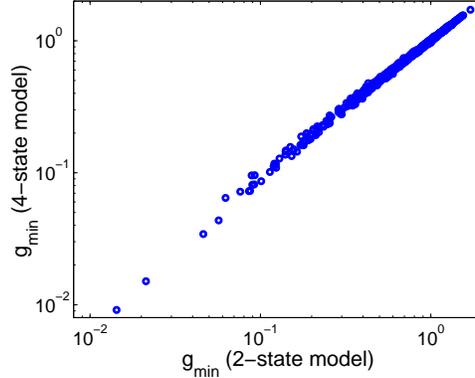
In a closed system, the computation time  $t_f$  is considered to be inversely related to the size of the minimum gap  $g_{\min}$  between the ground state and the first excited state. This gap is commonly obtained using the Hamiltonian of coupled ideal qubits, i.e., the first line of (6). Naively, one might think that adding the ancilla qubits would increase the total number of qubits and therefore would significantly reduce the size of the

minimum gap  $g_{\min}$ . One should keep in mind that the ancilla qubits are just added to model the upper energy levels that already exist in the spectrum of the actual physical device that plays the role of qubit. Therefore, the ancilla qubits should always be added if one wants to have a correct description of the real physical system. Since the number of upper energy levels are typically large, a large number of ancilla qubits is necessary to accurately describe all the energy levels. This means that even a small size system should be represented by a large number of qubits. Therefore, if the above statement is correct all realistic systems should have extremely small gaps. Intuitively, one expects that if the upper energy levels are far away from the lowest two levels, then their influence should be negligible. Thus, the presence of the ancilla qubits should not significantly affect the gap as long as  $\omega_p$  is much larger than other terms in the original Hamiltonian. As is clear from Fig. 1c,  $\omega_p$  is not very large, but still almost a factor of 3 larger than  $E(t)$  for the second half of the evolution. Therefore, it is expected that the excited levels, or equivalently the ancilla qubits, have some (but small) influence on the minimum gap and the evolution.

We test this conjecture by comparing the values of  $g_{\min}$  calculated with and without the ancilla qubits. To achieve this, we considered an ensemble of 8-qubit spin glass instances generated with random parameters:  $h$ 's and  $J$ 's were selected uniformly at random from  $0, \pm 1/7, \dots, \pm 6/7, \pm 1$ , except for  $J$ 's that don't represent an edge in the complete bipartite graph  $K_{4,4}$ , whose values were all zero. Among 800 instances generated, 669 of them had non-degenerate ground state for which we calculated  $g_{\min}$  using exact diagonalization technique. Figure 3 shows a comparison between  $g_{\min}$  calculated without the ancilla qubits (referred to as two-state model) and with the ancilla qubits (referred to as four-state model). As is clear from the figure, for some instances the size of the gap is increased and for some is decreased. On average the change of  $g_{\min}$  was below 1%. For the 4 data points available in the small gap region, the size of the gap was reduced by a maximum of 36%. More investigations, especially on larger problem instances, is necessary to determine if this is a trend for all small gap instances. Nevertheless, considering doubling the number of effective qubits from two-state model to four-state model, the above change is not significant.

## 4 Conclusions

The effect of the energy levels above the lowest two levels in the physical implementation of a qubit on adiabatic quantum optimization was



**Fig. 3.** Comparison of the minimum gap between two-state and four-state models.

studied. We discussed a model of a multi-level system with a double-well potential as a system of coupled qubits. One of the qubits (logical qubit) represents the logical state of the physical system and the remaining qubits (ancilla qubits) produce the upper energy levels. At the end of the evolution, the solution to the problem described by Hamiltonian  $H_P$ , is determined only by the state of the logical qubits. We showed that the state of the logical qubits in the final ground state is unaffected by the ancilla qubits, regardless of  $H_P$  (as long as potential bistability is preserved). Therefore, the same problems that can be solved by ideal qubits can also be solved using qudits. We studied the influence of the ancilla qubits on the minimum gap and showed that for realistic qubit parameters the effect for average problems is small. Problems with very small gap sizes had systematically smaller gaps when ancilla qubits were introduced into the formulation. However, the four data points in our simulation is not sufficient to predict a trend, especially for large scale problems. When generalized to open quantum systems using density matrix methods, the results of this model are in close agreement with results from experiments on a system of eight coupled rf-SQUID qubits. Discussion of the open quantum calculation and experiments is beyond the scope of this paper and will be discussed in a future publication.

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## Appendix: rf-SQUID Hamiltonian

In this appendix, we look closely at a specific example of qubit implementation, namely a compound Josephson junction rf-SQUID [7]. This choice was motivated by recent experimental progress in implementing multi-qubit quantum annealing process with such qubits [12]. All parameters for our numerical simulations are based on the 8-qubit unit cell studied in Ref. [12]. The qubit itself is discussed in detail in Ref. [7], but here we only consider a simplified version.

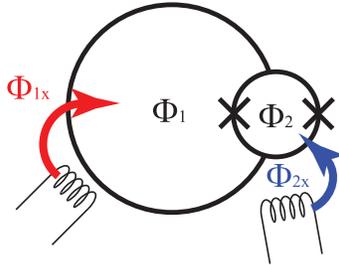
The qubit, as illustrated in Fig. 4, has two main superconducting loops and therefore two flux degrees of freedom  $\Phi_1$  and  $\Phi_2$ , subject to external flux biases  $\Phi_{1x}$  and  $\Phi_{2x}$ , respectively. The Hamiltonian of the qubit is written as

$$H_{\text{SQUID}} = \frac{q_1^2}{2C_1} + \frac{q_2^2}{2C_2} + U(\Phi_1, \Phi_2), \quad (7)$$

where  $C_1$  and  $C_2$  are parallel and series combinations of the junction capacitances,  $q_1$  and  $q_2$  are the sum and difference of the charges stored in the two Josephson junctions respectively, and

$$U(\Phi_1, \Phi_2) = (\Phi_1 - \Phi_{1x})^2/2L_1 + (\Phi_2 - \Phi_{2x})^2/2L_2 - 2E_J \cos(\pi\Phi_2/\Phi_0) \cos(2\pi\Phi_1/\Phi_0) \quad (8)$$

is a 2-dimensional potential with  $L_i$  being the inductance of the  $i$ th loop and  $\Phi_0 = h/2e$  is the flux quantum. We have assumed symmetric Josephson junctions with Josephson energies  $E_J = I_c \Phi_0 / 2\pi$ , where  $I_c$  is the junctions' critical current. (A small asymmetry can be tuned away in situ in the physical implementation [7].)



**Fig. 4.** Schematic diagram of a tunable rf-SQUID. The external fluxes  $\Phi_{1x}$  and  $\Phi_{2x}$  control the energy bias and tunneling amplitude respectively.

At  $\Phi_{1x} \approx \Phi_0/2$ , the potential can become bistable and therefore form a two-dimensional double-well potential. If  $L_2$  is small enough so that the deviation of  $\Phi_2$  from  $\Phi_{2x}$  can be neglected, then the two-dimensional classical potential  $U(\Phi_1, \Phi_2)$  can be approximated by a one-dimensional double-well potential, as shown in Fig. 1a. However, with our realistic qubit parameters,  $\Phi_2$  cannot be neglected and therefore is accounted for in all our numerical calculations. When  $\Phi_{1x} = \Phi_0/2$ , the two wells are symmetric with no energy bias ( $\epsilon = 0$ ). One can tilt the potential by changing  $\Phi_{1x}$  and establish an energy bias  $\epsilon$ , as depicted in Fig. 1a. It is also possible to change the barrier height by changing  $\Phi_{2x}$ . Quantum annealing is performed by slowly increasing the barrier height from a very small value to a very large value through ramping  $\Phi_{2x}$ . Details of the annealing process and techniques used to make all terms in the Hamiltonian change uniformly are discussed in Ref. [12]. At the end, the system behaves as the Hamiltonian (6) with all its time-dependent parameters determined experimentally. Our goal here is to extract these parameters numerically for the rf-SQUID Hamiltonian (7) having known all parameters ( $L_i, C_i, I_c$ ) and the experimental values of the external fluxes  $\Phi_{1x}(t)$  and  $\Phi_{2x}(t)$  as a function of time.

The eigenvalues  $E_n$  and eigenstates  $|E_n\rangle$  of the rf-SQUID Hamiltonian (7) can be calculated by numerical diagonalization. They, however, are not directly useful for simulations of AQO in a multi-qubit system defined by Hamiltonian (6). One therefore needs to derive (6), or single qudit version of it (2), from those eigenvalues and eigenstates. In principle, it is possible to write down the Hamiltonian in a basis defined by states  $|l\rangle$  localized in the wells, instead of the energy basis  $|E_n\rangle$ , as long as they form (at least approximately) an orthonormal basis. Our numerical procedure is as follows. First, we numerically diagonalize the original rf-SQUID Hamiltonian (7) to obtain energy eigenstates  $|E_n\rangle$ . We then select the first  $M$  eigenstates and diagonalize the flux operator  $\Phi_1$  in such subspace. This way we find  $M$  flux states  $|\chi_i\rangle$  with eigenvalues  $\chi_i$  each being a superposition of states  $|E_n\rangle$ . Some of the flux states will have negative and some positive induced flux  $\delta\Phi_i = \chi_i - \Phi_{1x}$ . We treat states with negative (positive) induced flux as states localized in the left (right) well. We then separate these two set of localized states and once again diagonalize the rf-SQUID Hamiltonian (7), but now separately in each left and right subspaces. The final result is a Hamiltonian that looks like (2). Different matrix elements of the resulting Hamiltonian determine different terms in (2) which in turn determine the parameters of the qudit Hamiltonian (3).