Adiabatic quantum optimization with qudits

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Abstract Most realistic solid state devices considered as qubits are not true two-state systems. If the energy separation of the upper energy levels from the lowest two levels is not large, then these upper states may affect the evolution of the ground state over time and therefore cannot be neglected. In this work, we study the effect of energy levels beyond the lowest two energy levels on adiabatic quantum optimization in a device with a double-well potential as the basic logical element. We show that the extra levels can be modeled by adding additional ancilla qubits coupled to the original logical qubits, and that the presence of upper levels has no effect on the final ground state. We also study the influence of upper energy levels on the minimum gap for a set of 8-qubit spin glass instances.

Keywords Adiabatic quantum optimization · Quantum annealing · Quantum computing

1 Introduction

The promise of revolutionizing the concept and possibilities of future computation has made quantum information processing (QIP) one of the fastest growing interdisciplinary research areas over the past decade [1]. In QIP, information is stored as quantum states of qubits, which are two-state quantum systems that represent...
the basic logical elements of quantum information. In practice, most realistic devices are not ideal two-state systems, so the ideal qubit model often used in QIP is only an approximation to the true quantum behavior of the device. For example, charge [2,3], hybrid [4], phase [5,6], and flux [7–11] qubits each have several energy levels, but only the lowest two energy levels are considered as the relevant qubit states.

The potential energy profile of a flux qubit is a double-well potential, similar to the one illustrated in Fig. 1a [7–11]. In the limit of infinite well barrier height, each well may be treated separately to obtain two sets of quantized energy levels localized within the wells. At finite barrier height, these localized states are no longer true eigenstates of the Hamiltonian. These states are metastable, which means a system initialized in one of these localized states will eventually transition out of it via tunneling. The true eigenstates of the Hamiltonian are coherent mixtures, or superpositions, of the localized states. Nevertheless, it is possible to represent the system in the basis of the localized states by introducing off-diagonal elements of the Hamiltonian, which provide tunneling amplitudes between states in opposite wells.

When the two lowest energy states dominate the dynamics of the system at low temperatures and small energy bias, one can consider the two-state system as a qubit. If the energy bias is comparable to the energy separations within each well, $\omega_p$, or the temperature of the system 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 each of these situations, one must include the occupied high 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 QIP is adiabatic quantum computation (AQC) [12,13] which is known to be a universal model of quantum computation [14,15]. In AQC, the dimensionless 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, when $E(0) \approx 0$, the dynamics are dominated by the Hamiltonian $\mathcal{H}_B$ and the ground state is generally a superposition...
of all states in the computation basis. At the end of the evolution, when \( \Delta(t_f) \approx 0 \), the dynamics are dominated by the problem Hamiltonian \( \mathcal{H}_P \), which is designed to solve the intended problem. If the evolution is sufficiently slow, then the final state of the system will represent the ground state of \( \mathcal{H}_P \) with high fidelity. The time-dependent energy scales \( \Delta(t) \) and \( E(t) \), usually not independent, are controlled by an external parameter. A typical example of functions \( E(t) \) and \( \Delta(t) \), based on a superconducting realization of the hardware [16], is provided in Fig. 1.

We focus on a special version of AQC known as adiabatic quantum optimization (AQO). AQO is also commonly referred to as quantum annealing [10,13,17,18], as it uses quantum fluctuations for annealing in a similar way as thermal fluctuations are used in classical annealing. In AQO, \( \mathcal{H}_P \) is diagonal in the logical basis. Therefore, the final ground state is a classical state that minimizes the energy, which can be considered as the optimized solution to a cost function. In this work, we are interested in the Ising Hamiltonian with transverse magnetic field,

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

where \( \sigma_x^{(i)}, \sigma_z^{(i)} \) are Pauli matrices corresponding to the \( i \)th qubit and \( h_i \) and \( J_{ij} \) are dimensionless energy biases and coupling coefficients, respectively. In this paper, we investigate how well an adiabatic quantum optimizer performs when using realistic qudits instead of idealized qubits.

The paper is organized as follows. In Sect. 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 this system by an effective tunneling Hamiltonian with finite number of levels and show how this can be represented by several coupled qubits. Then, we derive the parameters of the coupled qubit Hamiltonian representing the qudit in terms of the original tunneling Hamiltonian. In Sect. 3, we discuss how AQO is possible in a multi-qudit system and study the effect of extra energy levels on the minimum gap. Section 4 summarizes our results and conclusions.

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 the example of an rf-SQUID in the “Appendix”. We use 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 presented are expected to be in good agreement with experiments.

2 Single qudit Hamiltonian

Consider a system with a double-well potential similar to Fig. 1a. The Hamiltonian describing this model, written in the flux basis, has off-diagonal terms corresponding to
transitions between states in opposite wells. However, there are no off-diagonal terms corresponding to intra-well transitions, as these states are required 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 $n = 0, 1, 2, \ldots$ 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

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

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 opposite wells. Note that there is no matrix element between states within a well. Since $\langle 2n| H_S |2m\rangle = \langle 2n+1| H_S |2m+1\rangle = 0$, this means that these 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 derive the effective tunneling Hamiltonian for a bistable rf-SQUID and extract the parameters of this Hamiltonian from the original rf-SQUID Hamiltonian.

In a flux qubit, the direction of the flux generated by the persistent current in the superconducting loop identifies the well. At the end of the evolution, one measures the direction of magnetic flux 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”). It follows that all levels within a well are logically equivalent, which implies that the quantum numbers distinguishing states within a well are logically irrelevant. However, these degrees of freedom participate in the dynamics and must be taken into account in the quantum dynamics when studying the performance of the system.

In principle, there could be a large number of energy levels in the spectrum of the double-well potential. For example, assume that there are $M = 2^m$ relevant states. We express $l$ by its binary representation $x_{m-1} \ldots x_1 x_0$ and denote state $|l\rangle$ by $|x_{m-1} \ldots x_1 x_0\rangle$, with $x_i \in \{0, 1\}$, where $l = \sum_{i=0}^{m-1} 2^i x_i$. With the above even-odd representation of states, all states in 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). If $x_i$ represents the state of qubit $i$, then we have an effective system of $m$ qubits representing single qudit. However, in our qudit model, it is $x_0$ that determines the logical state of the system. We call this the “logical” qubit and refer to the remaining $m-1$ qubits as “ancilla” qubits.

In this work, we study the qudit model for a system of $m = 2$ qubits ($M = 4$). We denote states in the left potential well by $|00\rangle$ and $|10\rangle$ and states in the right potential well by $|01\rangle$ and $|11\rangle$. Note that each state can be represented by two coupled qubits. As shown in Fig. 1b, the bottom (top) qubit is 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 as $\sigma_\beta$. 

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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 is

$$H_{\text{eff}} = -\frac{1}{2} (\epsilon \sigma_z + \Delta \sigma_x) + \frac{1}{2} [\omega_p \tau_z + \kappa_{xz} \sigma_x (1 + \tau_z) + \kappa_{xx} \sigma_x \tau_x].$$  (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 levels by an energy difference equal to the plasma frequency $\omega_p$ ($\hbar = 1$). For $M = 4$, it is easy to show that Hamiltonian (3) is equivalent to Hamiltonian (2) up to a constant in energy, where

$$\epsilon = E_0 - E_1 = E_2 - E_3, \quad \omega_p = E_2 - E_0 = E_3 - E_1,$$
$$\Delta = -2 K_{01}, \quad \kappa_{xz} = K_{23} - K_{01} \approx K_{23}, \quad \kappa_{xx} = 2 K_{03} = 2 K_{12}. \quad (4)$$

The coupling between logical and ancilla qubits is type XX+XZ. Figure 1c shows typical values of these parameters during an annealing process based on the experimentally realized 8-qubit processor described in [16] (see the “Appendix”).

3 Adiabatic quantum optimization with qudits

We generalize our formulation to a system of coupled qudits. For flux qubits, the coupling is mediated via magnetic flux. In the multi-qubit representation, the state of the logical qudits represents the direction of the flux degree of freedom. Therefore, coupling via the logical qudits leads to a ZZ coupling term in the Hamiltonian. The role of ancilla qudits is a bit more subtle. Since the qudits are coupled via their flux degree of freedom, the ancilla qudits can participate in the coupling only if changing the state of the ancilla qudits affect the magnetic flux generated by the qubit. The ancilla qudit states determine whether the qubit is in the upper or lower state in a well. As we mentioned, within each well the direction of the flux is fixed and therefore does not depend on the state of the ancilla qubit. The magnitude of the flux generated, however, may depend on whether the rf-SQUID is in an upper state or lower state within a well. Therefore, in principle, ancilla qudits may also participate in the coupling Hamiltonian. In practice, however, the difference between the magnetic flux generated in the lowest state and the first excited state within a well is small. Therefore, the coupling between ancilla qudits, or between ancilla and logical qudits of different qudits, are neglected in our calculations. Of course, a more complete treatment can take into account these contribution, but the main conclusions of this paper will remain unaffected.

In order to recast the problem from a graph of coupled qudits into the form of coupled qudits, it is enough to connect an ancilla qudit to each qubit in the original problem via an XX+XZ coupling. Ancilla qudits are coupled only to their corresponding logical qudits; there is no coupling between the logical and ancilla qudits of other qudits. Figure 2 illustrates this situation for an example graph of four coupled qudits.
In the case of \( N \) qubits, the corresponding Hamiltonian is

\[
H_S = \Delta(t) \mathcal{H}_B + E(t) \mathcal{H}_P \\
+ \frac{1}{2} \sum_{i=1}^{N} \left[ \omega_p^{(i)}(t) \tau_z^{(i)} + k_x^{(i)}(t) \sigma_x^{(i)} (1 + \tau_z^{(i)}) + k_x^{(i)}(t) \sigma_x^{(i)} \tau_z^{(i)} \right].
\]

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 from the ancilla qubits.

Figure 1c shows the calculation of the parameters in 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, both the decrease of \( \Delta(t) \) and the increase of \( E(t) \) is monotonic in time. The non-monotonic variation of \( \omega_p \) represents the energy separation of the upper energy levels from the lowest two (see Fig. 1a). To approximate a qudit by a two-state qubit, the excited states within each well must be far above the lowest energy levels. This requirement puts a limit on the parameters of the problem Hamiltonian that \( h_i, J_{ij} \ll \omega_p/E(t) \). If this condition is not satisfied, the energy bias of the qubits may become so large that the energy of lowest state in one well approaches the energy of the excited state in the other well (see Fig. 1a as an example). In this situation, the two-state model is not applicable.

From Eq. 5 it is clear that the coupling coefficients between ancilla and logical qubits are related to tunneling amplitudes between opposite wells. At the end of the evolution, the barrier between the two wells becomes so large that tunneling between the lowest energy levels stops, meaning that all the off-diagonal elements of the Hamiltonian vanish, and \( \Delta = k_x^{(i)} = k_x^{(i)} = 0 \). This is clearly evident from our numerical calculation of these parameters in Fig. 1c. In the absence of such off-diagonal terms, the logical and ancilla qubits decouple and the ground state of the total Hamiltonian (6) is the ground state of \( \mathcal{H}_P \) for the logical qubits with all ancilla qubits being in state \( |0\rangle \). A residual coupling between the ancilla qubits, which can cause transitions within a potential well without going over the barrier, does not change such decoupling and therefore does not change the final state of the logical qubits. With this decoupling,
the ancilla qubits have no effect on the final ground state of the logical qubits even if $h_i, J_{ij} > \omega_p/E(t)$, but they still affect the dynamics of the system. This means that AQS 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 related to some inverse power of the size of the minimum gap between the ground state and the first excited state, $g_{\text{min}}$. Gap $g_{\text{min}}$ is obtained from the Hamiltonian of coupled ideal qubits, which is just the first line of (6). At first glance, it might appear that adding ancilla qubits increases the total number of qubits, which would then reduce $g_{\text{min}}$. We point out here that the ancilla qubits correspond to the upper energy levels that already exist in the spectrum of the device. Therefore, ancilla qubits should be included in order to have a complete description of the real system. It is necessary to include a large number of logical plus ancilla qubits to describe all energy levels accurately, which means that even small systems should be represented by a large number of qubits. This would seem to imply that all realistic systems will have extremely small gaps. However, if the upper energy levels are higher in energy than the lowest two levels, then their influence should be negligible and should not significantly affect the gap as long as $\omega_p$ is much larger than the other terms in the original Hamiltonian.

The issue of gap size is important when discussing the fidelity of the ground state in AQS as the system is evolved in time. As the gap size decreases, it becomes increasingly difficult to calculate the ground state of $\mathcal{H}_P$ at the end of the evolution. If upper energy levels within each qudit are important, then they should be included in any model in order to maintain a high degree of accuracy throughout the calculation. We test the effect of adding ancilla qubits by calculating $g_{\text{min}}$ with and without the ancilla qubits for an ensemble of 800 8-qubit spin glass instances. The random parameters $h$ and $J$ were selected uniformly at random from $0, \pm 1/7, \ldots, \pm 6/7, \pm 1$. The qudits’ connectivity was chosen to be a complete bipartite graph $K_{4,4}$, inspired by the experimental implementation [16]. Exact diagonalization of the spectrum currently inhibits us from moving to larger problem sizes at the moment. We are currently investigating ways to study larger system sizes with more energy levels per qudit as a focal point for future work.

Among all instances generated, 669 had non-degenerate ground states. We calculated $g_{\text{min}}$ for these instances using exact diagonalization. Figure 3 show the comparison between $g_{\text{min}}$ calculated for the two-state qubit model and the four-state qudit model. Although the size of $g_{\text{min}}$ varies with each instance studied, the change in $g_{\text{min}}$ is below 1% on average. For the four data points available in the small gap region, $g_{\text{min}}$ is reduced by a maximum of 36%. This suggests that $g_{\text{min}}$ does not change significantly as one moves from the qubit model to the qudit model. However, our data suggest that the ancilla qubits provide only a small correction for instances where $g_{\text{min}}$ is large, which leads to the conclusion that the standard qubit model is sufficient for studying AQS in these situations. More investigations, especially on larger problem instances, is necessary to determine if there is a trend for all small gap instances.
4 Conclusions

We investigated the effect of including energy levels above the lowest two levels in a qubit system on adiabatic quantum optimization using a model of a multi-level system with a double-well potential as a system of coupled qubits. In this model, the logical qubit represents the logical state of the physical system and the remaining ancilla qubits provide the upper energy levels. At the end of the evolution, the solution to the problem described by Hamiltonian $H_P$ is determined by the state of the logical qubits.

We have shown that the state of the logical qubits in the final ground state is unaffected by the ancilla qubits as long as potential bistability is preserved. Our results suggest that similar problems that can be solved by a qubit model can also be solved using a qudit model. Using qubit parameters obtained via experiment, we studied the influence of ancilla qubits on the minimum gap and showed that the solutions of average problems are robust against the inclusion of the upper energy levels. Although we found that problems with small gap sizes had systematically smaller gaps when ancilla qubits were introduced, the four data points in our simulation are not sufficient to predict a trend, especially for large scale problems. Unfortunately, increasing the size of the system studied, or increasing the number of levels kept in each qudit, would increase the total number of logical+ancilla qubits beyond 16, which is the limit of feasibility for exact diagonalization with the currently available computers. More elegant techniques have to be developed in order to study systems at larger scales. There are also other directions for further investigations. For example, one can investigate the role of the ancilla qubits on open system dynamics of the qudits, especially when the upper energy levels start to be thermally occupied. Open system results, using density matrix methods, from this model are in close agreement with results from experiments on a system of eight coupled rf-SQUID qubits [10].

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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 [9]. This choice was motivated by recent experimental progress in implementing multi-qubit quantum annealing process with such qubits [16]. All parameters for our numerical simulations are based on the 8-qubit unit cell studied in [16]. The qubit itself is discussed in detail in [9], 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

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

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

$$U(\Phi_1, \Phi_2) = (\Phi_1 - \Phi_{1x})^2/2L_1 + (\Phi_2 - \Phi_{2x})^2/2L_2 \tag{8}$$

$$-2E_J \cos(\pi \Phi_2/\Phi_0) \cos(2\pi \Phi_1/\Phi_0) \tag{9}$$

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 [9].)

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

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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.
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 [16]. 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).

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