Thermal Noise on Adiabatic Quantum Computation

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The success of adiabatic quantum computation (AQC) depends crucially on the ability to maintain the quantum computer in the ground state of the evolution Hamiltonian. The computation process has to be sufficiently slow as restricted by the minimal energy gap. However, at finite temperatures, it might need to be fast enough to avoid thermal excitations. The question is, how fast does it need to be? The structure of evolution Hamiltonians for AQC is generally too complicated for answering this question. Here we model an adiabatic quantum computer as a (parametrically driven) harmonic oscillator. The advantages of this model are (1) it offers high flexibility for quantitative analysis on the thermal effect, (2) the results qualitatively agree with previous numerical calculation, and (3) it could be experimentally verified with quantum electronic circuits.

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Adiabatic quantum computation (AQC) offers an alternative route for achieving computational goals [1], compared with the “standard model” of quantum computation based on the gate model. The basic idea of AQC is very simple: to maintain the system (computer) to stay at the (assumed unique) ground state with respect to a time-dependent Hamiltonian. For an isolated quantum system, this is in principle guaranteed by the quantum adiabatic theorem for sufficiently slow evolution, depending on the energy gap between the (instantaneous) ground state and the first excited state. Practically, AQC would be operated under some finite temperature which may not necessarily be negligible (recall energy gaps usually shrink with the increase of the problem size) compared with the energy gap. The effect of thermal noise would then play an important role in determining the performance of AQC. Physically, the relaxation process (i.e. excitation to higher energy states) takes finite time to complete. Hence, we expect that AQC needs to be sufficiently fast as well. This sets another time scale due to the environment. Consequently, unless thermalization is not an issue, AQC would work only if the computation time lies within these two time scales. The question is, how to determine the latter time scale involved? We shall answer this question in this letter.

This work is motivated by recent studies [2, 3, 4, 5, 6, 7, 8, 9] related to the question of robustness of AQC. Concerning the noise effect on AQC, some of the models are based on either qualitative or perturbative arguments which are not verified by independent numerical investigation. Some of them are formulated in terms of parameters which are inaccessible experimentally. On the other hand, it was believed [7, 8, 9] that two-level approximation would be valid for AQC, even if large number of excited states would be involved when the minimal gap is smaller than the temperature. It is therefore still unclear how “robust” AQC is against thermal noise.

With these problems in mind, our goal here is to study the thermalization problem of AQC by modeling a harmonic oscillator as a quantum computer. This model not only provides us with enough (infinite) excited states but also allows quantitative analysis. As we shall see, it could not be modeled by the two-level approximation. Moreover, we shall quantify the effects on the performance of AQC through physical quantities such as temperature $T$, relaxation time $1/\gamma$, energy gap $\Delta$ and computation time $\tau_c$. The “anomaly” of this model may seem to be the evenly distributed energy levels. To verify the validity, we have compared it with the numerical simulation by Childs et al. [2], and found that the predictions of this harmonic model qualitatively agrees with their results. Lastly, this model is testable with the current quantum electronic technologies, e.g. simple RLC circuits.

Adiabatic Quantum Computation — To define our adiabatic quantum computer, there are only two adjustable parameters, namely the “mass” $m_t \equiv m(t)$ and the “spring constant” $k_t \equiv k(t)$. The time dependence of these two parameters, at this stage, is completely arbitrary and is designed to simulate (e.g. see example III below) an adiabatic quantum computer. The (computational) system Hamiltonian $H_S(t)$ is described by that of a standard parametrically driven harmonic oscillator:

$$H_S(t) = \frac{p^2}{2m_t} + \frac{1}{2}k_t x^2,$$  \hspace{1cm} (1)

which is associated with a set of (instantaneous) energy eigenstates $|n_t \rangle$, with $n = 0, 1, 2, ...,$ satisfying the eigenvalue equation: $H_S(t) |n_t \rangle = E_n(t) |n_t \rangle$. Here $E_n(t) = (n + 1/2) \Delta(t)$ is the (instantaneous) eigenenergy for the state $|n_t \rangle$. The energy gap $\Delta(t) \equiv \sqrt{k_t/m_t} = E_{n+1}(t) - E_n(t)$ does not depend on $n$, by definition. The initial state is assumed to be the ground state $|0_{t=0} \rangle$ of $H_S(t = 0)$. In the absence of the heat bath, the final state is given by $U(t) (t = t_f) |0_{t=0} \rangle$, where

$$U(t) = \exp(-i \int_0^t H_S(t') dt') \quad \text{(with } \hbar = 1)$$

is a time-ordered series.

The computation is considered to be fail if the final
state deviates significantly (due to excitation to higher energy states) from the desired ground state \( |0_{t,f} \rangle \) of \( H_S \) \((t = t_f)\). This is best quantified by the fidelity \( F \equiv \langle 0_{t=f} | U(t_f) | 0_{t=0} \rangle \). Here since our goal is to study the thermal effect from the environment, we assume that AQC in the absence of the heat bath can be achieved (almost) perfectly, i.e., \( F \approx 1 \); violation of this condition may be considered as perturbation.

Under this condition (and to zeroth order in \( \Delta \) \((t)\)), we may write \( U(t) \langle n_0 \rangle = \exp(-i \int_0^t E_n(t') dt') \langle n_t \rangle \), and hence a relation which is needed later:

\[
U(t)a_t U(t) = \exp \left( -i \int_0^t \Delta(t') \ dt' \right) a_0 ,
\]

where \( a_t \equiv \sqrt{m_i \Delta_i/2} (\hat{x} + i \hbar / m_i \Delta_i) \) is the (instantaneous) annihilation operator for \( H_S(t) \).

**Ground State Occupation —** In the presence of a heat bath, a mixed state representation \( \rho(t) \), or the reduced density matrix \( \rho_S(t) = Tr_B \{ \rho(t) \} \), is needed. The performance of the quantum computer is determined by the ground state occupation \( P_g \equiv \langle 0_t | \rho_S(t) | 0_t \rangle \), and in the coordinate space:

\[
P_g = \int d^2x' dx \langle x' | \rho_S(t) | x' \rangle \varphi^*_1(x) \varphi_1(x') \ , \tag{3}
\]

where \( \varphi_1(x) \equiv \langle x | 0_t \rangle = (m_i \omega_i)^{1/4} \exp(-m_i \omega_i x^2/2) \) is the (instantaneous) ground state wavefunction of \( H_S(t) \). Before going into the technical details of the calculations for \( \rho_S(t) \), we first argue that, subject to the constraints \((a)\), \((b)\) and \((c)\) described below, the relevant quantity here is only the physical observable \( \langle \hat{x}(t)^2 \rangle \) (or the current fluctuation \( \langle 1(t)^2 \rangle \) in RLC circuits).

The imposed constraints are (a) the heat bath can be approximated by a set of harmonic oscillators \( H_B = \sum_k \hbar \omega_k b_k^\dagger b_k \), (b) the system-bath coupling \( \tilde{H}_{SB} \) is bilinear e.g., terms like \( \hat{x}(b_k + b_k^\dagger) \), and (c) the initial state of the bath is in a thermal state \( \rho_B = e^{-\beta_H \hat{H}_B} / Tr \{ e^{-\beta_H \hat{H}_B} \} \) and the system is in the ground state of \( H_S(0) \), i.e., \( \rho(0) = \langle 0_{t=0} | 0_{t=0} \rangle \otimes \rho_B \). To proceed, we write:

\[
| x' \rangle \langle x | = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\nu e^{i(\mu \nu - x^2)} e^{i(\mu \nu + \nu x)} , \tag{4}
\]

where \( \mu \equiv x - x' \) (and \( \nu \) is a just dummy variable). This form suggests that we have to evaluate the quantity \( \langle e^{i(\mu \nu + \nu^2)} \rangle \equiv Tr \{ e^{i(\mu \nu + \nu^2)} \rho(t) \} \), which is equal to \( \exp(-((\mu \nu + \nu^2)^2)/2) \) from the Bloch identity. Now, as verifiable by the master equation, here we claim that \( \langle a_2^2 \rangle = \langle a_1^2 \rangle = 0 \). By completing the Gaussian integrals in Eq. (3) and (4), we finally arrive at a very compact form for \( P_g \):

\[
P_g = \frac{1}{1 + n(t)} , \tag{5}
\]

where \( n(t) \equiv \langle a_1^\dagger a_1 \rangle = Tr \{ a_1^\dagger a_1 \rho(t) \} \). Thus, as advertised, \( \langle x^2 \rangle = (\hbar/2m_i \Delta_i) (2\langle a_1^\dagger a_1 \rangle + 1) \) is the only quantity needed to determine \( P_g \).

**Master Equation —** We shall obtain \( n(t) \) through the master equation approach [10]. Here the full Hamiltonian is divided into three parts: \( \tilde{H} = H_S(t) + H_B + \tilde{H}_{SB} \) where the first two terms have been defined. We assume that the coupling term \( \tilde{H}_{SB} \) is a time independent operator (i.e. independent of the mass \( m_t \) and spring constant \( k_t \) of the oscillator), and is explicitly given by:

\[
H_{SB} = \hat{x} \sum_k g_k (b_k + b_k^\dagger) . \tag{6}
\]

Note that there could be a frequency renormalization (lamb shift type), which modifies the ground state wavefunction. This effect would be small for weak damping \( \Delta(t) \gg \gamma(t) \) where \( \gamma(t) \equiv n(t) / m(t) \) (cf. Eq. (7) and (8)). Second, even for ohmic damping (time independent \( \eta(t) = \eta \)), the relaxation rate \( \gamma(t) \propto 1 / m(t) \) (or time to reach equilibrium) depends on the system parameter (here the “inertia” \( m(t) \)), and therefore may be time-dependent.

To continue, we shall keep the standard assumptions for the master equation, namely (i) product initial state, (ii) Born-Markov approximation (i.e. weak coupling and short memory time), and (iii) rotating wave approximation (i.e. ignore fast oscillations). Subject to these constraints, the master equation is given [10] by:

\[
\frac{d}{dt} \tilde{\rho}_S = -\frac{1}{\hbar^2} \int_0^t dt' Tr_B \{ [\tilde{H}_{SB}(t), \tilde{H}_{SB}(t')] \tilde{\rho}_S(t) \otimes \rho_B \} ,
\]

where in the interaction picture: \( \tilde{\rho}_S(t) = U(t)^\dagger \rho_S(t) U(t) \) and \( \tilde{H}_{SB}(t) = U(t)^\dagger \tilde{H}_{SB}(t) U(t) \). If we write \( x = \sqrt{\hbar/2m_i \Delta_i} (a_t + a_t^\dagger) \), and from Eq. (2), we obtain interaction terms similar to that of an ordinary (i.e. with mass and spring constant fixed) harmonic oscillator, except the replacement: \( \Delta_0 t \rightarrow \int_0^t dt' \Delta(t') \) and \( \rho(0) = \langle 0_{t=0} | 0_{t=0} \rangle \otimes \rho_B \). To proceed, we write:

\[
m(t) \frac{d^2}{dt^2} \langle x \rangle + \eta(t) \frac{d}{dt} \langle x \rangle + k(t) \langle x \rangle = 0 . \tag{7}
\]

The exception is the ohmic case, where \( J(\omega) \propto \omega \) and hence \( \eta(t) = \eta_0 \) is independent of the variation in the mass and the spring constant (e.g. RLC circuit). Finally, the equation for \( n(t) \equiv Tr \{ a_1^\dagger a_1 \rho_S(t) \} \) is obtained from the master equation:

\[
\frac{d}{dt} n(t) = -\gamma(t) (n(t) - N(t)) , \tag{8}
\]
where $N(t) \equiv 1/(e^{\Delta(t)/k_BT} - 1)$. This is the key result of this paper, since the performance of AQC is determined entirely by $n(t)$. Note that even for the case of ohmic damping, the relaxation rate $\gamma(t) \equiv \eta(t)/m(t)$ is in general time dependent. With the initial condition $n(0) = 0$, this equation can be solved numerically to obtain the ground state occupation $P_g$ at time $t$.

Although in our model the time dependence for the energy gap is completely arbitrary, for the purpose of understanding the structure of the thermal excitation we assume that the gap has a Landau-Zener type variation:

$$\Delta(t) = \sqrt{\Delta_{\text{max}}^2 (1 - t/\tau_s)^2 + \Delta_{\text{min}}^2}, \quad (9)$$

where for $\Delta_{\text{max}} \gg \Delta_{\text{min}}$, $\Delta(0) = \Delta(2\tau_s) \approx \Delta_{\text{max}}$, and $\Delta(\tau_s) = \Delta_{\text{min}}$. Except near the region $t \approx \tau_0$, the rate of change of the energy gap is $V_S \equiv \Delta_{\text{max}}/\tau_s$. For simplicity, we shall consider the ohmic case only and assume that $n(t) = n_0$ is time-independent, which makes $\gamma$ time-independent as well.

The following examples are chosen to demonstrate respectively that: (I) when thermalization is important (i.e. $\Delta(t) \leq k_BT$), the computation speed $V_S$ needs to be fast, compared with the “natural” speed of the bath $V_B \equiv \gamma k_BT$. We quantify this by defining $R \equiv V_B/V_S = \gamma k_BT/\Delta_{\text{max}}$. (II) After passing through the gap minimum, when the energy gap is larger than the temperature, i.e. $\Delta(t > \tau_s) > k_BT$, relaxation towards the ground state (increasing $P_g$) has the simple $e^{-\gamma t}$ dependence, and in contrast with that in Ref. [9], does not depend on $\Delta_{\text{min}}/\Delta_{\text{max}}$ in the exponent. (III) This toy model qualitatively agrees with numerical calculation based on more realistic Hamiltonian.

**Example I** — Consider the case where $\Delta_{\text{max}} \leq k_BT$ and $\Delta_{\text{min}} \ll k_BT$. It is possible to approximate $N(t) \approx k_BT/\Delta(t)$. Substitute this into Eq. (8), and with $\gamma(t) = \gamma$, we have

$$n(t) = \frac{\gamma k_BT}{\Delta_{\text{max}}} e^{-\gamma t} \int_0^t ds \frac{e^{\gamma s}}{(1 - s/\tau_s)^2 + \varepsilon^2}, \quad (10)$$

where $\varepsilon \equiv \Delta_{\text{min}}/\Delta_{\text{max}} \ll 1$. For $\gamma \tau_s < 1$, the integrand is dominated near $s \approx \tau_s$. Taking $e^{\gamma s} \to e^{\gamma \tau_s}$ and integrating explicitly, we have

$$n(t) = \lambda(t)Re^{-\gamma(t-\tau_s)}, \quad (11)$$

where $\lambda(t) \equiv \ln 2 - \ln[\sqrt{\varepsilon^2 + (1 - t/\tau_s)^2} + (1 - t/\tau_s)]$, and $R = \gamma k_BT/\Delta_{\text{max}}$ as defined above. Figure 1 shows that this expression for $n(t)$ is in good agreement with the result by direct numerical integration for $n(t)$. From Eq. (5), we conclude that the thermal effect is not important even if $\Delta(t) \leq k_BT$ provided that $\gamma \tau_s < 1$. More precisely, we require $R \ll 1$, or $V_S \gg V_B$. This minimal speed limit for AQC could not be seen by the two-level approximation [9].

![FIG. 1: Simulation of AQC with harmonic oscillator under thermal noise. The x-axis is rescaled time $\gamma t$. 1(a) and 2(a), in unit of $k_BT$, show the energy profiles Eq. (9) for two classes of AQC (but with the same $R$). 1(b) and 2(b) show the dynamics of the mean excitation of the oscillator. The solid lines are numerical integration from Eq. (8), and the dashed lines are analytic approximations Eq. (10) and Eq. (12). 1(c) and 2(c) are the corresponding ground state probabilities obtained from 1(b) and 2(b), with the relation Eq. (5). For comparison, the dotted lines are the thermal equilibrium values of $P_g = 1 - e^{-\beta \Delta}$.](image-url)
of \( \Delta_{\text{min}} \) in the exponent of \( n(t) \).

Example III — So far we have compared our results with that from the two-level approximation. Would a realistic Hamiltonian (with non-uniform distribution of energy gaps) for AQC, in some sense, look like a harmonic oscillator (uniform gaps)? If yes, then based on the results above, it may be possible to approximate the harmonic oscillator model (uniform gaps) for AQC, in some sense, look like a harmonic oscillator model. The results are shown in Table I. We extract, from FIG 2 of that paper, the final probability \( P_g \) and \( R \), and estimate the corresponding \( \alpha \) by the relation in Eq. (13), as suggested by our harmonic oscillator model. The results are shown in Table I. We then determine the (average) scaling \( \Gamma_n < 1 \) of the energy spectrum (typically the first few lowest energy states are enough). Then, to estimate the same AQC (under the same temperature) with large \( N \), the harmonic oscillator model suggests the ground state probability be given by the formula Eq. (13) with the replacement \( \Delta_{\text{max}} \to \Gamma N \Delta_{\text{max}} \) (assuming \( \tau_s \) and \( \gamma \) are fixed).

Conclusions — We have introduced a harmonic oscillator model for a quantitative study on the effect of thermal noise on AQC. For ohmic damping, we showed that AQC is considered fast, if the combination \( R = \gamma k_B T \tau_s / \Delta_{\text{max}} \) is small. This model suggests a simple relation for estimating the fidelity (cf. Eq. (13)) of general AQC; this relation qualitatively agrees with the previous numerical simulation. This model can also be verified with quantum RLC circuits, and therefore can act as a test bed for future theoretical and experimental investigation on AQC.

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### Table I: Simulation of AQC with Harmonic Oscillator

| \( k_B T \) | 1/10 | 1/2 | 2 | 10 |
|------------|------|-----|---|----|
| \( P_g \)  |      |     |   |    |
| \( \Delta_{\text{min}} = 0.301 \) | 0.79 | 0.53 | 0.30 | 0.15 | 0.08 |
| \( R \)    | 0.14 | 0.72 | 1.43 | 2.86 | 14.3 |
| \( \alpha \) | 1.86 | 1.24 | 1.63 | 1.98 | 0.80 |
| \( \Delta_{\text{min}} = 0.425 \) | 0.89 | 0.70 | 0.42 | 0.19 | 0.08 |
| \( R \)    | 0.17 | 0.87 | 1.74 | 3.48 | 17.4 |
| \( \alpha \) | 0.71 | 0.49 | 0.79 | 1.23 | 0.66 |

\( k_B T \) and \( \Delta_{\text{min}} \) are in unit of \( \Delta_{\text{max}} \).

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