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Thermally Assisted Adiabatic Quantum Computation

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We study the effect of a thermal environment on adiabatic quantum computation using the Bloch-Redfield formalism. We show that in certain cases the environment can enhance the performance in two different ways: (i) by introducing a time scale for thermal mixing near the anticrossing that is smaller than the adiabatic time scale, and (ii) by relaxation after the anticrossing. The former can enhance the scaling of computation when the environment is super-Ohmic, while the latter can only provide a prefactor enhancement. We apply our method to the case of adiabatic Grover search and show that performance better than classical is possible with a super-Ohmic environment, with no a priori knowledge of the energy spectrum.

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Quantum computation (QC) aims to harness the physical resources made available by quantum mechanics to gain an advantage over classical computation. A major obstacle to construction of a large scale quantum computer is loss of coherence resulting from uncontrolled coupling to the environment. In principle, environmental effects may be circumvented by the use of quantum error correction [1–4]. In practice, however, such schemes require significant overhead. It is therefore likely that many noisy qubits will be available before many error-corrected logical qubits are.

This observation motivates the search for models of QC with intrinsic resistance to noise. One such example is adiabatic quantum computation (AQC) [5–7]. Here we investigate a regime in which weak coupling to an environment can improve the performance of AQC.

In AQC, information is stored in the ground state of a quantum system and manipulated by control of the system Hamiltonian. An AQC is operated by deforming an initial Hamiltonian $H_i$ into a final Hamiltonian $H_f$ through intermediates $H_S = [1 - \lambda(t)]H_i + \lambda(t)H_f$, with $\lambda(t)$ changing from 0 to 1 between the initial ($t_i = 0$) and final ($t_f$) times. If the evolution satisfies the adiabatic condition ($h = k_B = 1$ throughout) $|\langle dH/\!\!d|0\rangle| \ll g^2(\lambda)$, where $g(\lambda)$ is the energy gap between the ground ($|0\rangle$) and first excited ($|1\rangle$) states, then the system will be in the ground state of $H_f$ at $t_f$ with probability close to 1, and the solution may then be read out [8]. In a global adiabatic scheme, $\lambda = t/t_f$ and the adiabatic condition must be satisfied for the smallest gap $g_m$. If $g(\lambda)$ is known, one can choose $d\lambda/dt \propto g^2(\lambda)$ to enhance the performance using a local adiabatic scheme [9]. Here, we assume no a priori knowledge of the energy spectrum, and use $\lambda = t/t_f$ throughout. The amount of time required to successfully run a computation is determined by the minimum gap between the first two energy levels, $g_m$, along the path connecting $H_i$ and $H_f$. In order for the evolution to remain adiabatic throughout, the total time required is $t_f \propto 1/g_m$.

Here we analyze the behavior of AQC in the presence of a thermal environment with temperature $T \gg g_m$. We restrict our analysis to problems in which the performance is limited by a single minimum gap of the type of an energy level avoided crossing. This corresponds to a first order quantum phase transition, which is believed to be hardest for AQC [10].

In general, if there are $l$ energy levels within the range $T$ from the ground state, then thermalization can suppress the ground state probability by at most a factor of $l^{-1}$. For a Gaussian distribution of the levels, $l$ is polynomial in the number of qubits $n$, if $T$ is much smaller than the total spectral width. In this case, one may compensate for thermalization by repetition with a polynomial overhead. Moreover, the transition times are expected to be very long, probably longer than the computation time, otherwise classical annealing would yield the solution efficiently. This is different from an anticrossing, at which point, as we shall see, the transition rate is sharply peaked. We therefore only focus on the anticrossing and use 2-level approximation.

Let us assume that the minimum gap occurs at $\lambda = \lambda_m$. We adopt a new coordinate, $\epsilon = 2E(\lambda - \lambda_m)$, where $E$ is an energy scale characterizing the anticrossing. Close to the anticrossing, the system Hamiltonian within the 2-level approximation is well described by

$$H_S = -(\epsilon \sigma_z + g_m \tau_z)/2,$$

and the gap between the first two states is well approximated by $g = \sqrt{\epsilon^2 + g_m^2}$. Here $\tau_{x,z}$ are the Pauli matrices in the 2-level subspace. Because of the Landau-Zener transition [11,12], the probability of being in the excited state at $t = t_f$ is given by

$$P_{1f} = e^{-t_f/t_a},$$

where $t_a = 4E/\pi g_m^2$ is the adiabatic time scale (see Table I for definition of all time scales).
We incorporate the environment by assuming that qubits are coupled to bosonic heat baths that are in equilibrium, with $g_m \ll T \ll E$. The total Hamiltonian is $H = H_S + H_B + H_{\text{int}}$, where $H_B$ and $H_{\text{int}}$ are bath and interaction Hamiltonians, respectively. We also assume that in the 2-level subspace the interaction Hamiltonian has the form

$$H_{\text{int}} = Q \otimes \tau_z,$$

where $Q$ is an operator representing the collective effect of all baths on the 2-state problem. Equations (1) and (3) capture the physics of a wide range of problems that have one sharp anticrossing.

For slow evolutions of the Hamiltonian considered here, as long as the correlation time of the environment is shorter than decay times of the system, one can safely assume Markovian approximation [13]. Writing the density matrix as $\rho = (1 + \rho \cdot \tau)/2$, the 2-state Bloch-Redfield equations are [14]

$$\dot{\rho}_x = -\gamma \rho_x + \epsilon \rho_y - \left( \frac{\epsilon}{g_m} \gamma - \frac{g_m}{\hbar} \gamma \right) \rho_z + \frac{g}{g_m} \rho_{\text{eq}},$$

$$\dot{\rho}_y = -\epsilon \rho_x - \gamma \rho_y + g_m \rho_z, \quad \dot{\rho}_z = -g_m \rho_y,$$

where $\gamma = (g_m/g)^2 [S(g) + S(-g)]$, $\gamma = 2(\epsilon/g)^2S(0)$, $\gamma = \gamma + \gamma \varphi$, and $\rho_{\text{eq}} = [S(g) - S(-g)]/[S(g) + S(-g)]$. Here, the bath's spectral density is defined as $S(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t}Q(t)Q(0)$, where $\langle \ldots \rangle$ denotes averaging over environmental degrees of freedom. The prefactor $(g_m/g)^2$ makes $\gamma$ sharply peaked at $\epsilon = 0$ as expected.

For a bosonic environment [15], $S(\omega) = J(\omega)/(1 - e^{-\omega/\omega_c})$, where $J(\omega) = \eta \omega_0 / \omega_c |e^{-\omega/\omega_c}|$, with $\omega_c$ being a cutoff frequency which is assumed to be larger than all other relevant energy scales in the system. Therefore

$$\gamma = (g_m/g)^2 J(g) \coth(g/2T), \quad \rho_{\text{eq}} = \tanh(g/2T).$$

Here, we focus only on Ohmic ($s = 0$) and super-Ohmic ($s > 0$) cases for which the correlation time of the bath $\sim 1/\omega_c$ is short compared to the relevant time scales. A sub-Ohmic ($s < 0$) environment has a large correlation time; hence, the Markovian approximation and therefore Bloch-Redfield equation do not hold [16].

We are interested in problems with small gap, $g_m \ll T \ll E$. We divide the evolution into three regions, as shown in Fig. 1. In region I, the gap is larger than $T$ and thermal transitions are suppressed. In region II, both thermal and nonadiabatic transitions between the two states are possible. In region III, the system again has a gap larger than $T$, but now the system can relax from the excited state to the ground state. Such relaxation can only increase the probability of success.

Let us start by finding the excitation probability immediately after region II. Assuming $T \gg g$, which holds for most of the region, we have $\rho_{\text{eq}} = 0$, and

$$\gamma = \gamma_0 \frac{g_m}{g^2} \left( \frac{g}{\omega_c} \right)^s, \quad \gamma \varphi = \left\{ \begin{array}{ll} \gamma_0 \epsilon^2/g^2 & \text{s = 0,} \\ 0 & \text{s > 0,} \end{array} \right.$$

where $\gamma_0 = 2\eta T$. We perform the calculation in the regime $g_m \ll \gamma$. The presence of the damping terms in the first two equations in (4) will make $\rho_x$ and $\rho_y$ decay in a time scale $\sim 1/\gamma$ much shorter than the relevant time scale for $\rho_z \sim 1/g_m$. Thus, to find the slow evolution of $\rho_z$, one can use the stationary values for $\rho_x$ and $\rho_y$, obtained from $\dot{\rho}_{x,y} = 0$. Solving the first two equations in (4) for $\rho_y$ and substituting into the third equation, we get

$$\dot{\rho}_z = -\Gamma(\epsilon)\rho_z, \quad \Gamma(\epsilon) = g^2 \gamma/(\gamma^2 + \epsilon^2).$$

Here, $\Gamma$ is the rate of transition between the two branches of energy that meet at the anticrossing. Integrating (7), we find

$$\ln \frac{\rho_z(t)}{\rho_z(0)} = - \int_0^t d\epsilon \Gamma(\epsilon) = - \int_{-T}^{e(t)} \frac{d\epsilon}{\epsilon} \Gamma(\epsilon),$$

which leads to

$$\rho(\epsilon = T) = \rho(0)e^{-t_f/\tau_d},$$

where $t_f$ is a characteristic time scale that describes the thermal mixing near the anticrossing, and is given by

$$\frac{1}{\tau_d} = \frac{1}{t_f} \int_{-\infty}^{\infty} \frac{d\epsilon}{\epsilon} \Gamma(\epsilon).$$

We have taken the integration limits to infinity assuming that $\Gamma(\epsilon)$ is sharply peaked at $\epsilon = 0$, which is the case for $s < 1$. Using the initial condition $\rho_z(0) = 1$, the excitation probability after region II is approximately

$$P_x(\epsilon = T) = \frac{1}{2}(1 + e^{-t_f/\tau_d}).$$

For a linear time evolution (i.e., $\lambda = t/t_f$), one has $\epsilon = 2E/t_f$. If the environment is Ohmic, then $s = 0$ and $\gamma = \gamma_0$ is a constant. Therefore
in agreement with Kayanuma [17] and Ao and Rammer [18]. For fast evolutions (short \( t_f \)), (11) behaves the same way as a closed system (2), while in the slow regime (long \( t_f \)), (11) gives a ground state probability of \( \sim 1/2 \), corresponding to the complete mixture of the two states.

For a super-Ohmic bath (\( s > 0 \)), \( \gamma_\varphi = 0 \), hence \( \tilde{\gamma} = \gamma = \gamma_0 (g_m/g)^3 (g/\omega_s)^3 \). In such a case,

\[
\frac{1}{t_d} = \frac{1}{2E} \int_{-\infty}^{\infty} d\epsilon \frac{\Lambda g^4}{\Lambda^2 g^{2\epsilon^2} + \epsilon^2},
\]

where \( \Lambda = \gamma_0 g_m^2 / \omega_s^2 \). The important contribution to the integral comes from regions with \( g = |\epsilon| \sim \Lambda^{1/(3-s)} \gg g_m \), where the inequality follows from \( g_m \ll \gamma_0 (g_m / \omega_s)^s = \tilde{\gamma}(0) \), which was our initial assumption. This condition, however, can be satisfied in the limit of \( g_m \to 0 \), only if \( s < 1 \). Replacing \( \epsilon = \Lambda^{1/(3-s)} \xi \), we find

\[
t_d = \alpha_s E \left( \frac{\omega_s^2}{2 \gamma_0 g_m^2} \right)^{2/(3-s)}, \quad \frac{1}{t_d} \approx \int_0^{\infty} \frac{x^{1-s} dx}{1 + x^{3-2s}}.
\]

Since \( \alpha_s \) is independent of \( g_m \), we have \( t_d \propto g_m^{-4/(3-s)} \) which scales better than \( t_d \sim g_m^{-2} \). It is easy to check that the integral is convergent for \( s < 1 \). For \( s > 1 \), the condition \( g_m \ll \tilde{\gamma} \) cannot be satisfied in the limit of \( g_m \to 0 \), invalidating our approach.

We now study the effect of relaxation after the anticrossing (region III). From (7), we see that \( \Gamma(\epsilon \gg \tilde{\gamma}) = \gamma \). The probability of ending up in the excited state becomes \( P_1(\epsilon = E) = P_1(\epsilon = E) e^{-\int_t^\infty \gamma de / \epsilon} \). Using (5) and assuming \( \coth(g/2T) = 1 \), which holds for most of the region, and \( \epsilon \gg g_m \), we find

\[
\frac{1}{2E} \int_T^E \gamma de = \frac{\eta g_m^2}{2E \omega_s^4} \int_T^E e^{s-1} de = \frac{1}{t_r}.
\]

Here we have defined a third time scale \( t_r \), that characterizes such a relaxation process. One can write \( t_r = t_d/\kappa_s \), where

\[
\kappa_s = \frac{2 \eta}{\pi} \left[ \ln(E/T) \right] \left[ \frac{1}{2} (E/\omega_s)^2 - (T/\omega_s)^2 \right] = 0,
\]

Notice that \( t_r \) slowly decreases with \( T \).

The probability of success, i.e., the final ground state probability, is therefore given by

\[
P_{0f}(t) = 1 - \frac{1}{2} \left( 1 + e^{-t/s} \right) e^{-t/r}.
\]

It reaches \( \sim 1/2 \) in a time \( t_f \sim t_d \), but approaches 1 in a time \( t_f \sim t_s \). If \( t_d < t_s \), it is advantageous to run the system faster but repeat the process. The relevant time scale for computation will then be \( \sim 2t_d \), which for an Ohmic environment is \( \sim t_d \propto g_m^{-2} \), the time scale for a closed AQC.

On the other hand, for super-Ohmic cases with \( 0 < s < 1 \), one has \( t_d \propto g_m^{-4/(3-s)} \), which shows an improved performance compared to the closed AQC, as \( g_m \to 0 \). The performance becomes better as \( s \) gets closer to zero, until \( s = 0 \) (i.e., Ohmic) at which point the low frequency part of the noise spectrum becomes nonzero and the performance goes back to \( 1/g_m^4 \).

This sudden change at \( s = 0 \) is related to the sharp jump in \( S(\omega) \propto \omega^{1/2} \) at \( \omega = 0 \), from a nonzero value at \( s = 0 \) to zero at \( s > 0 \). However, the \( S(0) \) that appears in the definition of \( \gamma_\varphi \) is not exactly zero frequency, but really the low frequency component of the noise, i.e., \( S(\sim 1/t_f) \). As \( s \) becomes smaller, the low frequency component gets larger and eventually dominates the \( \tilde{\gamma} \) in (8), resulting in a smooth transition to the Ohmic behavior. Without the \( S(0) \) term, an Ohmic environment would yield a \( t_d \propto g_m^{-4/3} \) behavior. Here, a competition between pure relaxation, which tends to enhance the performance, and pure dephasing (due to the low frequency noise) which works against it, is noticeable. Taking both processes into account, in the case of Ohmic environment, the performance of the system will be the same as that for a fully coherent AQC.

For systems with \( t_d > t_r \), the computation time scale will be determined by \( t_r \) and the ground state probability, for small \( t_f \), will basically have the form \( P_{0f}(t) \approx 1 - e^{-t/t_f} \). If \( t_f < t_r \), then we will again have a better performance compared to a closed AQC. However, as we saw before, \( t_r \) has the same \( g_m^{-2} \) dependence as \( t_s \). Thus, any speedup over AQC by this process can only be via a prefactor \( \kappa_s \) (if it is larger than 1). The enhancement reported in Ref. [7] falls in this category since the number of qubits considered was not large enough to obtain small \( g_m \) and therefore thermal mixture at the anticrossing.

We should emphasize that Eq. (16) is calculated assuming that the 2-state approximation holds for the entire range. While this can be the case for some Hamiltonians, such as adiabatic Grover search [9], it is not true in general. In fact, it is very difficult to calculate \( t_r \) for a general problem. However, one would not expect this type of relaxation, which is equivalent to classical annealing, to give any scaling benefit over classical computation.

We now apply our approach to the adiabatic implementation of Grover’s search algorithm [9,19]. In this case, the explicit dependence of \( g_m \) on the problem size may be obtained, and hence all quantities may be calculated in terms of the size of the unstructured search problem \( N = 2^n \). Following Roland and Cerf [9], we use the Hamiltonian \( \hat{H}_g = E[\mathbb{1} - (1 - \lambda) \hat{\Omega}(+) + \hat{\Omega}(+) \hat{\Omega}(\lambda) \hat{\Omega}(m)] \), where \( \{|m\} \) is the marked state to be found and \( |\pm\rangle = (N^{-1/2} \sum_i |i\rangle \). Defining \( \epsilon = E(2\lambda - 1) \), the gap is \( g(\epsilon) = \sqrt{\epsilon^2/N + (1 - 1/N) \epsilon^2} \). The minimum gap, \( g_m = E/\sqrt{N} \), lies at \( \epsilon = 0 \). The third energy level, \( E_2 = E \), has \( (N-2) \)-fold degeneracy. A global adiabatic algorithm \( \lambda = t/f_f \) results in \( t_f \sim N/E \) [20]. Using a local adiabatic algorithm [9], one can achieve \( t_f \sim \sqrt{N}/E \). Because of the large degeneracy of \( E_2 \), the 2-level approximation will only be valid in the temperature regime \( T \ll E/\log N \).
We consider the implementation of the unstructured search problem on \(n\) qubits, and hence may describe our noise model in terms of operators acting on these qubits. We show that the type of 2-level noise model (3) indeed arises for a general coupling of qubits to the environment: 

\[
H_{\text{int}} = -\sum_{i=1}^{n} (X_i \otimes \sigma_i^x + Z_i \otimes \sigma_i^z),
\]

where \(\sigma_i^a\) are the Pauli matrices for the \(i\)th qubit, and \(X_i, Z_i\) are its corresponding heat bath operators. In the large \(N\) limit, the effective 2-level system and interaction Hamiltonians become (1) and (3), respectively, where \(Q = \frac{1}{2} \sum_i (X_i - Z_i)\).

Assuming uncorrelated heat baths, (17) also holds for this problem with \(\eta = \frac{1}{2} n (\bar{\eta}^+ + \bar{\eta}^-)\), where \(\bar{\eta}^\pm\) are average friction coefficients for the \(X_i\) and \(Z_i\) operators.

For large \(n\), the scaling of \(t_d\) with \(N\) is given by \(t_d \sim N\) for Ohmic, and \(t_d \sim N^{2/(3-s)}\) for super-Ohmic environment (with linear interpolation). It is clear that for super-Ohmic environment with \(s < 1\), the scaling is better than that for classical computation.

We have also performed numerical simulations of adiabatic Grover search, solving the Bloch-Redfield equations without the 2-level or large \(N\) assumption for 12, 16, and 20 qubits. Figure 2 plots \(P_{\text{off}}\) as a function of \(t_f/t_a\) for a case with super-Ohmic environment with \(s = 0.5\). As is clear from the figure, the curves increase faster compared to a closed system for larger \(n\) (smaller \(g_m\)). This agrees with the scaling advantage of the noisy system compared with the closed system according to our analytical prediction.

To summarize, using the Bloch-Redfield formalism we have identified 3 time scales for the evolution of AQC and determined their scalings with \(g_m\). We have shown that relaxation after the anticrossing can only provide a prefactor enhancement for computation time. Thermal mixing at the anticrossing, on the other hand, can enhance the scaling of the computation if the environment is super-Ohmic with \(0 < s < 1\), while the same environment will be destructive for gate model QC. This underlines the important difference between the two models in response to the environment. Finally, we should mention that a presence of low frequency noise, as in spin environment [21], will remove the above enhancement.

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