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Kibble-Zurek mechanism in simulated annealing and quantum annealing

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Abstract. We study errors of quantum annealing and simulated annealing to highlight better performance of quantum annealing over simulated annealing. Quantum annealing and simulated annealing perform optimization through a quantum adiabatic evolution and a quasi-static evolution respectively. In both methods, dynamics across a phase transition plays a crucial role. The Kibble-Zurek mechanism is known as an underlying physics of defect formation during a time-evolution across a phase transition. We apply an argument for the Kibble-Zurek mechanism to the error generation of quantum annealing and simulated annealing. We show that, for the disordered Ising chain, the kink density and residual energy per spin of quantum annealing decay as \((\ln\tau)^{-2}\) and \((\ln\tau)^{-4}\) respectively, whereas those of simulated annealing decay as \((\ln\tau)^{-1}\) and \((\ln\tau)^{-2}\) with the annealing rate \(-1/\tau\). These results imply better performance of quantum annealing. We also develop our theory for a two-dimensional spin-glass model.

1. Introduction
Solving optimization problems is not only the main topic in computer science but also an important subject in condensed matter physics [1]. Several methods have been proposed for optimization problems from the physicist’s point of view. Simulated annealing is an algorithm which is applicable to generic optimization problems and uses the notion of statistical mechanics [2, 3]. Quantum annealing is another generic algorithm [4, 5, 6, 7, 8, 9]. Quantum annealing applies the quantum mechanics for classical problems. A great question is whether the quantum mechanics is able to make speed-up from the classical algorithm in computation. In this paper, we focus on a comparison of quantum annealing and simulated annealing.

Let us consider an Ising model: \(H_{\text{Ising}} = \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z\), where \(\sigma_i^z\) is the Ising spin and \(J_{ij}\) is the coupling constant. If \(J_{ij}\) is disordered, the ground state of this Hamiltonian can be non-trivial and difficult to find. For instance, there is no known algorithm to find the ground state of the three-dimensional spin-glass model in a polynomial time with system size [10]. A lot of optimization problems, including the travelling salesman problem, satisfiability problem, and so on, can be mapped to such ground-state search problems of a disordered Ising model. Simulated annealing offers an approximate solution to these problems. In simulated annealing, one introduces a fictitious temperature and makes a thermal equilibrium state by means of the Monte-Carlo simulation or molecular dynamics simulation. When \(T\) is sufficiently high, it is easy to realize the equilibrium state, but it is not for low \(T\). At first we make the equilibrium state at high \(T\) and then decrease \(T\) with time. If the decreasing speed of \(T\) is sufficiently slow, the distribution of spin states changes with keeping the equilibrium distribution at each temperature.
and the ground state is obtained with high probability in the end when the temperature becomes zero. Quantum annealing, on the other hand, introduce the transverse field, $-{\Gamma}\sum_{i}\sigma_{x}^{i}$, instead of the temperature, where $\sigma_{x}^{i}$ is the $x$-component of the Pauli’s spin operator and $\Gamma$ stands for the strength of the field. At first we set $\Gamma$ at a sufficiently high value and make the ground state. This ground state is easily made since all spins are aligned along the transverse field. Then we decrease $\Gamma$ with time. If the decreasing speed of $\Gamma$ is sufficiently slow, the spin state evolves adiabatically and reaches the ground state of $H_{\text{Ising}}$ when $\Gamma$ vanishes. Quantum annealing is naturally implemented in the quantum computer. However, it is possible to implement in the classical computer if one uses the quantum Monte-Carlo method. In this case, the Schrödinger dynamics is replaced by the stochastic dynamics of the Monte-Carlo method.

Both in simulated annealing and quantum annealing, the phase transition is an obstacle to the success. Consider a thermodynamic phase transition. In the vicinity of phase transition, the relaxation time diverges, and hence the distribution of spin states cannot keep track of the Gibbs-Boltzmann’s distribution as far as the temperature is decreased with a finite rate. As for a quantum phase transition, the energy gap $\Delta$ between the ground state and the first excited state vanishes at the critical point. Since the adiabatic condition with changing $\Gamma$ is given by $|\dot{\Gamma}|/\Delta^{2}\ll 1$ [9, 11], the adiabaticity breaks at the critical point. The Kibble-Zurek mechanism is known as an underlying physics of defect formation during such a dynamics across a phase transition [12, 13]. By applying the Kibble-Zurek argument to simulated annealing and quantum annealing, we explicitly derive scaling formulas with respect to the error after annealing for one-dimensional disordered Ising model. In fact, we show that the densities of kinks after simulated annealing and quantum annealing are scaled as $\rho^{\text{SA}}\sim (\ln \tau)^{-1}$ and $\rho^{\text{QA}}\sim (\ln \tau)^{-2}$ respectively, where $-1/\tau$ is the annealing rate. We also show that residual energies per spin are $\epsilon_{\text{res}}^{\text{SA}}\sim (\ln \tau)^{-2}$ and $\epsilon_{\text{res}}^{\text{QA}}\sim (\ln \tau)^{-4}$. These results reveal that quantum annealing reduces the error faster than simulated annealing at least for the disordered Ising chain.

We organize this paper as follows. In the next section, we explain the Kibble-Zurek mechanism in detail. We then apply the argument of section 2 to the disordered Ising chain in section 3. The main results of this paper is presented here. In section 4, we discuss a two-dimensional system. Although we have not reached definite results on a two-dimensional system, we provide a hint which may be useful in future work. This paper is concluded in section 5.

2. Kibble-Zurek mechanism

Let us consider a ferromagnet with the critical temperature $T_{c}$. In the standard second order phase transition, the correlation length $\xi$ and the relaxation time $\tau_{r}$ increase with decreasing temperature toward $T_{c}$ as $\xi\sim \epsilon^{-\nu}$ and $\tau_{r}\sim \xi^{z}\sim \epsilon^{-z\nu}$, where $\epsilon = (T-T_{c})/T_{c}$ is the dimensionless temperature, and $z$ and $\nu$ are critical exponents.

Now we consider quenching temperature with time $t$ as $T(t) = T_{c}(1-t/\tau)$, namely, $\epsilon(t) = -t/\tau$, where $-1/\tau$ is the quench rate and we assume that the time moves from $-\infty$ to $\tau$. We assume that the system is in its equilibrium state initially. As far as the temperature is sufficiently high and the relaxation time is sufficiently short, the system can maintain its equilibrium with decreasing temperature. However, when the temperature becomes close to $T_{c}$, the temperature decreases further before the system attains the equilibrium. Thus the system cannot achieve the ferromagnetic long-range order and contains ferromagnetic domains when the temperature goes below $T_{c}$. Once the domain structure forms, it would not vanish since a large energy barrier lies between this state and the uniformly ordered state. The size of the domain is estimated as follows. We focus on two scales of time in our system. One is the remaining time $|t|$ to the critical point, and the other is the relaxation time $\tau_{r}$. We then equate them:

$$\tau_{r} = |t|.$$  \hspace{1cm} (1)

This equality defines the time $\hat{t}$ at which the relaxation time is equal to the remaining time to the
critical point. Since \( \tau_c = \epsilon / \nu = (|t|/\tau)^{-\nu} \), one obtains \( \hat{t} = \tau^{\nu/(\nu+1)} \). After the time passes \( \hat{t} \), the system never attains the equilibrium since the relaxation time is longer than the remaining time. Suppose here that the system stays in the equilibrium at \( \hat{t} \equiv \epsilon(\hat{t}) = \tau^{-1/(\nu+1)} \) and does not evolve any more after \( \hat{t} \). Then the correlation length of the state after \( \hat{t} \) is approximated by \( \xi \equiv \xi(\hat{t}) = \tau^{\nu/(\nu+1)} \). This gives an estimate of the size of the domain produced by quenching temperature. The density of defects can be estimated by \( \rho \sim \hat{t}^{-d} \), where \( d \) is the dimension of the system. Therefore one obtains \( \rho \sim \tau^{-\nu/(\nu+1)} \).

3. Disordered Ising chain
In this section, we focus on simulated annealing and quantum annealing of the disordered Ising chain. The Hamiltonian of the disordered Ising chain is given by

\[
\mathcal{H}_{\text{Ising}} = - \sum_i J_i \sigma_i^z \sigma_{i+1}^z. \tag{2}
\]

In the present study, we assume that \( J_i \) obeys the uniform distribution between 0 and 1, namely, \( P(J_i) = 1 \) for \( 0 \leq J_i \leq 1 \) and \( P(J_i) = 0 \) otherwise. The ground state of this model is obviously the state with the complete ferromagnetic order. However the excited states reflect the randomness in the coupling constants, which influence annealing dynamics.

3.1. Simulated annealing
The disordered Ising chain does not show the phase transition at any finite temperature. The critical temperature is regarded as \( T_c = 0 \). We assume that the temperature is decreased as \( T = -t/\tau \) with time moving from \( t = -\infty \) to 0. We employ the Glauber’s model \([14]\) for the spin dynamics.

Let us apply the argument in section 2 to this system. At first, the correlation function between two spins is obtained as \( \langle [\sigma_i, \sigma_{i+r}] \rangle = (\ln \cosh \beta/\beta)^r \) in the thermodynamic limit, where \( \langle \cdots \rangle \) stands for the average with respect to the distribution of \( J_i \) and \( \beta \) is the inverse of the temperature. From this, the correlation length for \( T \ll 1 \) is obtained as

\[
\xi \approx \beta/\ln 2. \tag{3}
\]

Next, the relaxation time under the Glauber’s model is given by \([15]\)

\[
\tau \approx \frac{1}{2} e^{4\beta} \approx \frac{1}{2} e^{(4 \ln 2)\xi}. \tag{4}
\]

The scaling properties of this zero-temperature phase transition is different from those of the standard second order phase transition. Hence we return to equation (1). From equations (3) and (4) with \( \beta = -\tau/t \), one obtains an equation of \( \xi : \frac{1}{2} \exp[(4 \ln 2)\xi] = \tau/(\xi \ln 2) \) which yields

\[
\hat{\xi} = \frac{1}{4 \ln 2} \left( \ln \tau - \ln \frac{\xi \ln 2}{2} \right). \tag{5}
\]

Note that we write the solution of the equation of \( \xi \) as \( \hat{\xi} \). For \( \tau \gg 1 \), this reduces to \( \hat{\xi} \approx \ln \tau/(4 \ln 2) \). The inverse of the correlation length provides an estimate of the density of kinks in the Ising chain:

\[
\rho^{\text{SA}} \approx \frac{1}{\xi} \approx \frac{4 \ln 2}{\ln \tau - \ln(\xi \ln 2/2)}, \tag{6}
\]

which reduces to \( \rho^{\text{SA}} \sim (\ln \tau)^{-1} \) for \( \tau \gg 1 \). Since the kink is seen as the error against the ferromagnetic ground state, this result implies that the error of simulated annealing decays as \( 1/\ln \tau \) with increasing \( \tau \).
The residual energy is also an important quantity in measuring the error. The energy expectation value per spin at low temperature is given by
\[ \langle E \rangle = \frac{1}{2} + \frac{\pi^2}{24} \beta^{-2}, \]
where the first term corresponds to the ground-state energy. This expression with equations (3) and (5) leads us to an estimate of the residual energy per spin:
\[ \varepsilon_{\text{res}}^{\text{SA}} \approx \frac{2\pi^2}{3} \left( \ln \tau - \ln \frac{\xi \ln 2}{2} \right)^{-2}, \] (7)
which reduces to \( \varepsilon_{\text{res}}^{\text{SA}} \sim (\ln \tau)^{-2} \) for \( \tau \gg 1 \).

The analytic results on \( \rho^{\text{SA}} \) and \( \varepsilon_{\text{res}}^{\text{SA}} \) obtained above have been supported by numerical simulation [16].

### 3.2. Quantum annealing

To study quantum annealing of the disordered Ising chain, we consider the following Hamiltonian:
\[ \mathcal{H} = \mathcal{H}_{\text{Ising}} - \Gamma \sum_i h_i \sigma_i^z, \] (8)
where \( h_i \) is a random constant which is introduced for calculational convenience. \( h_i \) obeys the same probability distribution as \( J_i \). This model exhibits a quantum phase transition at \( \Gamma = 1 \) [17]. For \( 0 \leq \Gamma < 1 \), the ground state is ferromagnetic, i.e., \( \langle \sigma_i^z \rangle > 0 \). On the other hand, the paramagnetic ground state is realized for \( \Gamma > 1 \). The quantum critical point at \( \Gamma = 1 \) of this model is called the infinite randomness fixed point. Its property has been revealed by means of the strong disorder renormalization group [17, 18, 19, 20]. Let us write the distance from the critical point as \( \epsilon = \Gamma - 1 \). The correlation length is scaled with \( \epsilon \) as
\[ \xi \sim |\epsilon|^{-\nu}. \] (9)

What makes this quantum phase transition unusual is that the distribution of the energy gap \( \Delta \) above the ground state at the critical point is scaled by \( -\ln \Delta/L^\psi \) using the system size \( L \) and an exponent \( \psi \). Hence the coherence time \( \tau_{\text{coh}} \), defined by the inverse of the averaged energy gap, is scaled with \( \xi \) as
\[ \ln \tau_{\text{coh}} \sim \xi^\psi. \] (10)
The exponents \( \nu \) and \( \psi \) have been obtained as \( \nu = 2 \) and \( \psi = \frac{1}{2} \) [17, 18]. These scaling properties are the same in the case with \( h_i = 1 \) for all \( i \).

Now we assume the time-dependent transverse field: \( \epsilon = -t/\tau \), where \( t \) moves from \( -\infty \) to \( \tau \). We follow the argument of section 2 starting from equation (1). Taking the logarithm of equation (1) and using (9), (10) and \( |t| = \tau \epsilon \), one has
\[ \hat{\xi}^\psi \sim \ln(\tau \xi^{-1/\nu}), \] (11)
which reduces to \( \hat{\xi} \sim (\ln \tau)^{1/\psi} = (\ln \tau)^2 \) for \( \tau \gg 1 \). Therefore one obtains the density of kinks after quantum annealing as \( \rho_{\text{QA}} \sim (\ln \tau)^{-2} \) [21, 22].

The scaling of residual energy after quantum annealing is estimated as follows. Suppose that there is one kink per length \( L \) in the chain. The smallest coupling constant in the chain of length \( L \) is estimated as \( 1/L \). Hence the energy cost per spin coming from the kink is given by \( 1/L^2 \). Now the state after quantum annealing should be the state with correlation length \( \hat{\xi} \). This implies that there is one kink per length \( \hat{\xi} \) on average. Therefore the residual energy per spin is estimated as \( \varepsilon_{\text{res}}^{\text{QA}} \sim 1/\hat{\xi}^2 \sim (\ln \tau)^{-4} \).

The result on the density of kinks has been supported by numerical simulation [22]. As for the residual energy, numerical simulation has produced \( \varepsilon_{\text{res}}^{\text{QA}} \sim (\ln \tau)^{-3.4} \) on the basis of results for sizes up to 512 spins [22]. We expect that this discrepancy is due to finite size effects.
Figure 1. Residual energies after simulated annealing and quantum annealing of the two-dimensional spin-glass model with 99 x 99 spins. Simulated annealing and quantum annealing are performed by the classical and quantum Monte-Carlo methods [28] respectively. Simulated annealing is started from an initial temperature $T = 5.0$ and quantum annealing is done from $\Gamma = 5.0$ at $T = 0.01$. The uniform transverse field is applied in quantum annealing. The random average is taken over 100 runs for a single sample for simulated annealing and single run for 16 samples for quantum annealing. The decay of the residual energy of simulated annealing is well fitted by $(\ln \tau)^{-2}$. For quantum annealing, the residual energy decays approximately as $(\ln \tau)^{-3}$ except for long $\tau$ where it has a slower decay rate. The decay rate for quantum annealing is faster than simulated annealing. However, its rate is different from $(\ln \tau)^{-4.47}$ obtained theoretically.

4. Spin-glass in two dimension

The disordered Ising chain we studied in the previous section has the trivial ground state. It is significant to discuss the case with a non-trivial ground state. Here we consider the two-dimensional spin-glass model: $H_{\text{Ising}} = \sum_{<ij>} J_{ij} \sigma_i \sigma_j$, where $J_{ij}$ obeys the uniform distribution between $-\Delta$ and $\Delta$. For simulated annealing of spin-glass systems, the Huse-Fisher law provides the upper bound $(\ln \tau)^{-2}$ for the decay rate of the residual energy [23]. In fact, as shown in figure 1, numerical results are well fitted by $\xi_{\text{res}}^{\text{SA}} \sim (\ln \tau)^{-2}$. The Huse-Fisher law is independent of the Kibble-Zurek mechanism and originates from spin dynamics of a small spin cluster. Hence this fact implies local spin dynamics dominates the error of simulated annealing. As for quantum annealing, there is no known mechanism like the Huse-Fisher law. In the presence of the transverse field, the quantum phase transition of this model should be characterized by the infinite-randomness fixed point [24], like in one-dimension. Hence, the same argument as the previous section yields $\xi \sim (\ln \tau)^{1/\psi}$. In order to estimate the residual energy, we assume that a lowlying droplet excitation from the ground state in a system with size $L$ in the absence of the transverse field costs an energy $L^\theta$ [25], namely $L^{\theta-d}$ per spin, where $\theta$ is the stiffness exponent and $d$ is the dimension of the system. Then, with the correlation length $\xi$ after annealing, the residual energy per spin should be scaled as $\xi_{\text{res}}^{\text{QA}} \sim \xi^{\theta-d} \sim (\ln \tau)^{(\theta-d)/\psi}$. Unfortunately we have no estimates for $\theta$ and $\psi$ so far. However, if one substitute the value $\theta \approx -0.29$ of the Gaussian spin-glass [26] and $\psi \approx 0.48$ of the random transverse Ising ferromagnet [27], one reaches $(\theta - d)/\psi \approx 4.77$. In figure 1, we show results of the quantum Monte-Carlo simulation. It is clear that the decay of residual energy after quantum annealing is faster than simulated annealing. However one finds that $\xi_{\text{res}}^{\text{QA}}$ behaves almost as $(\ln \tau)^{-3}$ which is slower than $(\ln \tau)^{-4.77}$ except for long $\tau$ where it has a still slower decay rate. One of the reason of this disagreement
might be the difference between the Schrödinger dynamics and the Monte-Carlo dynamics. However, since our scaling analysis is independent of the detail of the rule of dynamics, our theoretical result may be applicable to the Monte-Carlo dynamics. Next, one can attribute the disagreement to the values of $J_{ij}$ we used. The uniform distribution of $J_{ij}$ may produce different $\theta$ from the Gaussian distribution. Moreover it is not clear whether the frustration is irrelevant or not at the infinite-randomness fixed point. Finally, there is a possibility that another unknown mechanism dominates the decay of residual energy. To clarify the nature of quantum annealing in non-trivial systems, we need analytic and numerical studies further.

5. Conclusion
We studied residual errors after simulated annealing and quantum annealing with the particular attention to the Kibble-Zurek mechanism. For the disordered Ising chain, simulated annealing produces the density of kinks and residual energy per spin which are scaled as $\rho_{\text{SA}} \sim (\ln \tau)^{-1}$ and $\varepsilon_{\text{res}}^{\text{SA}} \sim (\ln \tau)^{-2}$, whereas quantum annealing produces $\rho_{\text{QA}} \sim (\ln \tau)^{-2}$ and $\varepsilon_{\text{res}}^{\text{QA}} \sim (\ln \tau)^{-4}$. These scaling relations are confirmed numerically except $\varepsilon_{\text{res}}^{\text{QA}}$ for which we ascribed the discrepancy to finite size effects of simulation. Our results on decay rates of residual errors reveal better performance of quantum annealing in comparison with simulated annealing. We also discussed the two-dimensional spin-glass model. Although we presented theoretical and numerical results, further studies are needed to clarify the discrepancy between them.

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