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Review

Quo Vadis quantum annealing?

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Abstract. In this article we sketch a broad outline of quantum annealing as a framework for realizing analog quantum computation. We provide a short review of the basic ideas and discuss some issues relevant to the current scenario of condensed matter physics and quantum computation.

1 Classical annealing

Annealing is an age-old technique of producing defect free crystals from the melt by slow cooling. Slower the rate of cooling is, lesser is the number of defects. The rationale is, if the cooling is quasi-static then the system always remains in equilibrium at the instantaneous temperature (T) and form a perfect crystal (defect density will vanish in the infinite size limit) when the temperature is reduced to zero. If the cooling is not quasi-static then the molecules do not get enough time to arrange themselves in configurations conforming with the equilibrium state at the instantaneous temperature due to local jamming and blockages, and defects are generated as a result. How slow is slow enough? The simple qualitative answer is, the cooling rate should be slower than the slowest relaxation process in the system. The slow timescales of relaxation often arise due to existence of metastable states (local free-energy minima) surrounded by free-energy barriers, where the system gets trapped. Given sufficient time, thermal fluctuations eventually get the system out of such metastable states and bring it to the actual equilibrium (one of the global free-energy minima). If the temperature is decreased slow enough such that the system is always at equilibrium with the instantaneous temperature, then the system will be found in one of its global potential energy minimum as $T \to 0$. This natural technique inspired a simple but brilliant heuristic framework, namely simulated annealing for optimizing complex multi-variate cost functions [1]. The essence is to treat the variables in the problem as physical degrees of freedom, the cost function to be minimized as the potential energy, and adopt a time-dependent artificial temperature T that gives the necessary thermal fluctuations. One can choose, e.g., the probability $P(E_i \to E_f)$ of going from a configuration of cost E_i to E_f ($E_f > E_i$) proportional to $\exp[-(E_f - E_i)/T]$.

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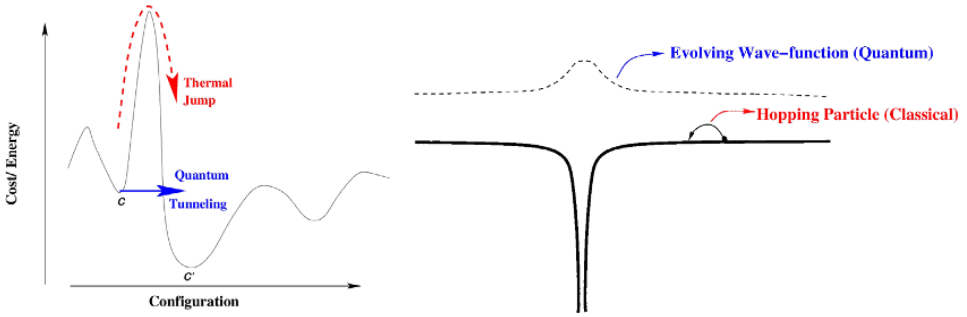

Fig. 1. Cartoon illustrating two scenarios in which quantum annealing might be better than thermal annealing. Left frame showing quantum tunneling might help exploring the potential energy landscape more easily when hindered by high but narrow barriers. Right frame shows a quantum particle with a wave-function delocalized over the entire potential energy landscape can "feels" a deep isolated potential minimum (hole) on a flat potential energy landscape (table) even before "falling" (completely localizing) into it. This is an analog version of the Grover's search problem.

One then begins with an equilibrium state at very high temperature – the "melt", and slowly reduce T to zero following some annealing schedule. During the process the system is simulated using a suitable Monte Carlo scheme. The temperature allows the system to explore the energy landscape effectively by helping it getting out of the shallow local energy minima, where simple gradient descent type of algorithms would get stuck. The success of simulated annealing is overwhelming due to its generic nature, easy implementability, and effectiveness in finding well-optimized solutions for several problems of practical interest.

2 Quantum annealing

However, there can be scenarios where search using thermal fluctuations might fail miserably in principle. In some of those, one might expect search using quantum fluctuations could considerably improve the situation. In the following we discuss two such scenarios in retrospect.

(I) *Exploring a Landscape with Lofty but Narrow Energy Barriers*: In order to cross a potential energy barrier by thermal excitations, a classical system has to "jump" over the barrier, i.e., acquire a (kinetic) energy equal to or greater than the barrier height. If T is the temperature, then the probability of acquiring such a kick is suppressed exponentially as a function of the barrier height h_B: $P_{cross} \propto \exp[-h_B/T]$. This poses a serious problem if there are high barriers around a local energy minimum. The thickness of the barrier does not appear in P_{cross} and hence even a narrow barrier can trap a system for long time if it is high. But the situation is quite different for a quantum system tunneling through an energy barrier. For a given incident energy (whose characteristic scale is given by T), the probability P_{tunnel} of tunneling through a barrier of a given height is higher if the barrier is thinner, quite in contrast to what happens in the classical case (see, e.g., [2]). Hence for a barrier of a given height, quantum tunneling would always be the easier way to cross it than to jump over it thermally if it is narrow enough (Fig. 1, left frame).

In certain classical systems, namely, classical spin glasses, where quenched disorders and frustrations in the interaction between the spins are strong, there are local free-energy minima which are surrounded by free-energy barriers whose heights scale

with the system-size N. In those systems the metastable states surrounded by such barriers becomes as stable as actual equilibrium states, implying a randomly broken ergodicity [3]. The two key elements behind the glassy behaviour, namely, disorder and frustration, are also generic in many challenging optimization problems.

It was conjectured in late 80's that, due to quantum tunneling, such a classical spin glass could become ergodic in presence of a quantum term (one which does not commute with the classical spin-glass Hamiltonian) of finite strength [4]. Though the domain of validity of the above conjecture is not yet known, the superiority of quantum tunneling over thermal jumps in crossing narrow enough barriers is still one reason behind the hope for improvement in search algorithms using quantum fluctuations instead of the classical ones in some cases.

(II) *Exploring a Flat Landscape*: In optimization using classical fluctuations, at each instant the system is in one of the "classical" configurations of the system, defined by a set of *definite* values of the variables and the cost function. But in the quantum version of the search problem, all the classical configurations together form a complete set of basis states in the Hilbert space, and the system is allowed to be in simultaneous superposition of an arbitrary number of them. This ability of a quantum system to access and process several configurations which are mutually exclusive classically, is known as "quantum parallelism" in the literature of quantum computation [5]. This endows one with certain computational edges which no classical computer can enjoy. Below we provide a simple illustrative example.

Consider a flat table with a hole somewhere on it and a particle moving on the table. Everywhere on the table, the potential energy (due to gravity, say) is constant, while right at the hole it is lower. If the particle is classical, it will have no clue about the hole unless it falls right into it. Hence the time for a classical particle to find the hole on an average cannot grow slower than linearly with *area* of the table, i.e., the dimension of the Hilbert space (we have of course discretized the *area* of the table in units of the size of the area of the hole). The point is, this average time does not depend on the depth of the hole. In fact, since there is no potential gradient, thermal annealing, or for that matter, no classical search protocol can do any better than a random search in this case.

But a quantum particle with a wave-function delocalized over the table can "feel" the depth of the hole at any given instant, as illustrated in Fig. 1 (right frame). Thus, the depth of the hole is expected to affect the search time on an average (this non-classical role of the strength of the potential energy in reducing the search time for an infinite range hopping has in fact been demonstrated; see [6]). It was shown in the said work, that if the depth of the hole is kept proportional to the area of the table, then the quantum search time will be of $\mathcal{O}(1)$, i.e. independent of the area of the table. Increasing the depth of the hole will not however affect the time required for any classical searcher to find it in any way. The above search problem is a version of Grover's problem [7] of searching an unstructured data-base (discussed further in a later subsection), but used for illustrating a bit different aspect of quantum speed-up.

2.1 Quantum annealing in classical computers

The idea of using quantum tunneling instead of thermal jumps to formulate improved stochastic optimization search schemes for combinatorial problems came in late 80's [8]. The idea of quantum annealing, i.e., performing annealing using quantum fluctuations (see [9,10] and [11] for review) for optimizing multi-dimensional functions [12,13] or hard combinatorial problems [14] came in 1990's. In those works low but finite temperature quantum Monte Carlo dynamics was used for simulating quantum annealing, of course, in classical computers. The objective was to determine the ground state of

a d-dimensional classical Hamiltonian H_c. The annealing scheme consisted of adding a quantum part H_q of time-dependent coupling strength $\Gamma(t)$ ($[H_c, H_q] \neq 0$). H_q is so chosen that (a) its ground-state is known and easily realizable (b) it is a roughly equal superposition of all classical configurations. The total Hamiltonian at any instant is thus

$$H_{tot} = H_c + \Gamma(t) H_q.$$

At $t = 0, \Gamma(0) \gg 1$, i.e., $H_{tot} \approx H_q$, and the initial state is prepared at the equilibrium state of H_q. Then Γ is slowly reduced with time. The dynamics of the system is simulated by mapping the d-dimensional quantum system to a $d+1$-dimensional classical system using, say, Suzuki-Trotter mapping (see, e.g., [15]). Annealing ends when the Γ reaches zero, and one is left with the classical Hamiltonian H_c at its low temperature equilibrium or a deep metastable state. The temperature is finally annealed to zero. The entire process forms a heuristic search algorithm, and one is likely to get a good approximation to the most optimal configurations through this process. Remarkable success of quantum annealing over simulated annealing in finding low energy configurations of certain 2d spin-glasses using finite temperature quantum Monte Carlo was reported [16]. A zero temperature quantum Monte Carlo based algorithm was also formulated and applied successfully to small instances of an NP-complete problem [17]. Faster relaxation of a quantum spin system induced by quantum annealing was also demonstrated experimentally [18].

2.2 Adiabatic quantum computation

In the year 2000, based on adiabatic theorem of quantum mechanics (see. e.g., [19]), a version of quantum annealing, known as adiabatic quantum computation was formulated [20,21]. The dynamics is assumed to be Schrödinger evolution, and hence is expected to be carried out in a "quantum annealer" or an analog quantum computer [9].

Quantum parallelism and Grover's algorithm: A crucial feature which makes quantum computation superior to classical computation, namely, quantum parallelism, is achieved only when one runs quantum annealing on a quantum computer. A system with n degrees of freedom can be in $N \sim \mathcal{O}(e^n)$ number of classical configurations. If any search/simulation requires evaluating all of those, then no classical computer can bypass expenses of $\mathcal{O}(N)$ – either in terms of computation time or in terms of computational resources to accomplish the task. On contrary, as illustrated above, quantum parallelism allow some kind of access of all these $\mathcal{O}(N)$ configurations simultaneously. But there is a catch. While in a superposition of several configurations, the system "feels" the characteristics of each configuration very weakly (proportional to its Born weight in the superposition), and hence extracting information about a state with a desired property is not a trivial task. As a matter of fact, there is no guarantee that one can even in principle build a search algorithm based on this, which will outperform any classical search algorithm in general. But there are at least few cases, where this can be guaranteed. One illustrative example is the Grover's problem, where, in essence, there is a list of N random objects (which can be labeled using integers encoded in $n \sim \log N$ quantum bits or qubits), and one has to search if any entry on the list satisfies some pre-assigned search criteria. Since checking a particular entry does not give any clue about the other entries, no classical sampling algorithm will do better than a random search which will require resources (run-time/queries/processors) $\mathcal{O}(N)$ on an average (recall the problem of searching a hole on a flat landscape). But it was shown by Grover [7] that clever use of quantum parallelism allows one to solve this search problem employing only $\mathcal{O}(\sqrt{N})$ resources. Quantum Annealing version

of Grover's algorithm was formulated later [22]. Thus the hole can be found within a time that scale as $\sqrt{area}$ of the table using quantum annealing using Grover's idea.

2.3 Exponentially small gap – A major bottleneck for quantum annealing

In adiabatic quantum annealing, the rate of the annealing required to ensure reaching the ground state end is bounded from below by the minimum gap $\Delta_{\min}$ between the instantaneous ground state and the low-lying excited state(s) of the time-dependent Hamiltonian over the entire annealing time. Unfortunately, in most cases of practical interest, $\Delta_{\min}$ is exponentially small in system-size n. This implies accurate annealing would require an exponentially large annealing time. Moreover, there seems to be no way to guess how $\Delta_{\min}$ will scale with n in general, from broad characteristics of the problem at hand. For example, though in most cases first order phase transitions $\Delta_{\min} \sim e^{-n}$ at the transition point as our intuition might suggest (see the article by Suzuki in this issue), this cannot be a rigorous fact, and interesting exceptions has been discovered recently incorrect [23,24]. Both power-law and exponential scaling of $\Delta_{\min}$ was observed depending on parameters of the Hamiltonian at a first order phase transition point. Exponentially small gap, however, seems to be a generic feature of the spectrum of a system with quenched disorders. Below we touch upon the basic ideas, since such disorders are unavoidable in our daily lives and hence in most of the optimization problems we are interested in.

Anderson localization and exponentially small gap due to disorder: Let us consider the problem of a single quantum particle searching for the global potential-energy minimum in a strongly disordered potential energy landscape. Here annealing is done by tuning the kinetic energy (1/effective mass) of the particle from a very high value to zero with time. If the disorder is strong enough, then for some definite value of the effective mass there will be an Anderson transition to a localized phase, where (at least) the low-lying states are localized in small regions in the real space. It was argued that is such cases, quantum annealing must fail due to occurrence of exponentially small $\Delta_{\min}$ in the localized phase [25]. Below we reconstruct a version of that argument.

Let us consider two different potential wells W_0 and W_1 in the potential energy landscape separated spatially by a large distance ξ. Let those be the deepest (W_0) and next deepest (W_1) wells in the landscape. Thus our search is aimed to find W_0. In the limit of complete separation (zero probability of tunneling from one well to the other), let $|\psi_0\rangle$ and $|\psi_1\rangle$ denote the ground state wave functions of the wells W_0 and W_1 with ground state energies ϵ_0 and ϵ_1 respectively. If W_0 is deeper than W_1, then $|\psi_0\rangle$ and $|\psi_1\rangle$ will respectively be the ground state and first excited states of the joint system of two (unconnected) wells (assuming $\epsilon_1 - \epsilon_0$ is much smaller than the gap between the ground states and the excited states of respective wells). But in presence of non-zero kinetic energy and a finite separation ξ, the ground state and the first excited state of the joint system will approximately be given respectively by the ground state $|\mathrm{Gr}\rangle$ and first excited state $|1_{ex}\rangle$ of the two level Hamiltonian

$$H_{AL} = \epsilon_0|\psi_0\rangle\langle\psi_0| + \epsilon_1|\psi_1\rangle\langle\psi_1| + \tilde{\Gamma}|\psi_0\rangle\langle\psi_1| + \tilde{\Gamma}^*|\psi_1\rangle\langle\psi_0|,$$

where $\tilde{\Gamma}$ denotes the off-diagonal tunneling term. Note that $\tilde{\Gamma}$ is not the global parameter that can be tuned to anneal the system, like. e.g., the disorder strength (though it depends on the tuning parameter). If the system is in the Anderson-localized phase, then smallest relevant values of $\tilde{\Gamma}$ will typically be exponentially small in system-size, as the tunneling between wells separated by macroscopic distances will be relevant to

maintain adiabaticity, and the tunneling between the wells are suppressed exponentially with the separation between them. Thus close to the transition point, quantum annealing has to be slowed down exponentially in system-size, so that a significant transfer of probability density from W_1 to W_0 can take place for all relevant cases. In particular, when kinetic energy is large, ground state tends to have greater overlap with the broader wells. Hence if the deepest wells are much narrower compared to the characteristic width of the wells, a lot of probability current has to flow to those as the transition point is neared, in order to follow the instantaneous ground state. In such a case exponential slowing down near the transition is a must to secure any useful approximation.

Disorder without frustration: Presence of both frustration and quenched disorder in a Hamiltonian/cost function makes the problem of finding its ground state hard. Disorder without frustration is however an easy problem, since in absence of frustration, the cost can be minimized locally. But for quantum annealing, even such benign disorders can prove fatal. For example, it was shown that finding the ground state of a 1D classical random Ising Hamiltonian of L spins, which can be obtained just by inspection (choose the 1st spin at random, then choose the second one to satisfy the bond between the first and the second, choose the third to satisfy the bond between the second and the third, and so on), can take sub-exponential (i.e. $\sim e^{L^{\epsilon}}$, where ϵ is a number independent of L) time when approached via quantum annealing using a transverse field as the source of fluctuations [26]. The reason is again appearance of sub-exponentially small gaps: $\Delta_{min} \sim e^{-\sqrt{L}}$.

2.4 Quantum annealer as an efficient quantum simulator

Simulation of non-equilibrium dynamics: Exact calculation of properties of a quantum system using a classical computer requires resources which grows exponentially with system-size n, since the dimension of the Hilbert space associated with it has an exponential growth. In many cases, however, mapping a d-dimensional quantum system to a $d+1$ dimensional classical system, allows for very accurate simulation of equilibrium properties of a quantum system via Monte Carlo simulation of the corresponding classical system. But simulating real-time (Schrödinger) dynamics of the system has still remained an exponentially difficult task in general. In some special cases certain results can be derived correctly from imaginary-time Monte-Carlo dynamics, e.g., certain universal features of the dynamics in case of slow annealing across a quantum critical point [27], but in general extracting accurate information about the real-time evolution from any imaginary-time dynamics via analytic continuation is hard (see, e.g. [28]).

Dynamics of an open quantum system are of more practical importance and also are much more difficult to simulate. In particular, the dynamics induced in a subsystem of a closed quantum system due to its interaction with the rest of the system (bath) are often of great interest, particularly in context of quantum computation and quantum information processing devices (see, e.g. [5]). Understanding how a well isolated quantum hardware loses its coherence and energy due to minimal coupling with its surroundings is a major practical issue in the field of quantum engineering. But since a bath is itself a quantum system, typically much larger than the subsystem under consideration, the overhead of simulating the total system of (subsystem + bath) accurately is even larger than simulating the dynamics of the subsystem if it were closed. There are certain special situations where simplistic formalism like Lindblad formulation or stochastic Schrödinger equation can give reasonable results (see, e.g., [29]), but those are only ad hoc methods based on several simplifying assumptions

about the characteristics of the bath and the system which are hard to verify in general. Hence accurate simulation of the dynamics of open quantum system has long remained in its infancy.

But with a proper quantum annealer, this blockade can be removed trivially. Simulating non-equilibrium dynamics is equivalent to allowing the system to evolve with time under certain initial conditions and possibly under an external drive. The exponential number of states participating in the dynamics are automatically accessed by the hardware as a superposition of all of them. Thus, in effect, a quantum annealer solves a set of an exponential number of coupled partial differential equations with a time-dependent Schrödinger operator in parallel. To simulate an open quantum subsystem, the total system to be simulated is the (subsystem + bath). Here of course the term "quantum annealer" is used in a broader sense – it means a quantum system whose couplings can be tuned in a controlled way, and is protected from unwanted decoherence and dissipation to a desired degree (which of course are some of the basic criteria to be satisfied even by a conventional quantum annealer in general).

Simulating physics of disorder free frustrated systems: In context of physical systems, frustration means presence of competing interactions or constraints, all of which cannot be satisfied simultaneously by any configuration of the system. Presence of frustrations in interacting quantum systems is the key to a plethora of exotic and interesting phases of matters, like quantum spin-liquids (see, e.g. [30,31]). Emergence of objects like fractional excitations and effective gauge-fields in those systems has put quantum frustration to one of the major focuses of the present day condensed matter research. But there are serious difficulties in simulating such frustrated systems on a classical computer using quantum Monte Carlo. The problem is as follows. Consider a d-dimensional quantum system, mapped to a $d+1$-dimensional classical system, say, via Suzuki-Trotter decomposition. One can expect to reproduce the properties of the quantum system by simulating the mapped classical system (of course, truncated after some finite but sufficiently large extent in the Trotter direction). Now consider a given set of basis states $\{|b_i\rangle\}$, representing, say the complete set of classical configurations of the $d+1$-dimensional classical system. In this basis, the canonical equilibrium average of a physical quantity $\mathcal{A}$ will be represented by

$$\langle \mathcal{A} \rangle = \frac{\sum_i \mathcal{A}(|b_i\rangle) P(|b_i\rangle)}{\sum_i P(|b_i\rangle)},$$

where $P(|b_i\rangle)$ represents the "weight" of the configuration $|b_i\rangle$ in the effective $d+1$-dimensional partition function. If the quantum Hamiltonian is frustrated, say because of fermionic exclusion principles (see, e.g., [32]) or due to competing interactions between the spins (see, e.g. [33]), then the weights $P(|b_i\rangle)$ obtained from the quantum to classical mapping may be negative, or even complex. In order to carry out the Monte Carlo anyway, an ad hoc remedy could be to replace $P(|b_i\rangle)$ by $|P(|b_i\rangle)|$ and interpret those as probabilities. But doing so leads to a relative error (in estimating the averages) that grows exponentially with the number of degrees of freedom. This problem is generically known as the sign-problem. This has kept the numerical studies of quantum spin-liquids and other interesting quantum frustrated systems severely restricted only to exact methods like exact diagonalization, best of which can afford to go only up to sizes of few fundamental lattice units for $d \geq 2$ (see, e.g., [34]).

But using a quantum annealer, ground states and low energy manifolds of such systems can be explored efficiently in many cases of prime interest. This is because in those cases the inverse of the minimum spectral gap $1/\Delta_{\min}$ encountered during quantum annealing are upper-bounded by polynomials in system-sizes. An illustrative

example is spin-1/2 Kagome-Heisenberg antiferromagnet, which is a hallmark spin-liquid candidate (see, e.g., [34]).

Simplicity of the analog format of quantum computation: Last but not the least, for employing quantum computation for quantum simulation and solving combinatorial optimization problems, the quantum annealing format seems to be the most natural choice. For quantum simulation of physical systems, one needs to construct the Hamiltonian in question by tailoring the coupling between the basic degrees of freedoms and tuning the couplings with time. This is becoming increasingly easier to achieve in laboratories for several paradigmatic condensed matter systems due to stupendous rate of progress in development of experimental techniques, most importantly, in the field of cold atoms in optical lattice [35]. As far as combinatorial optimization problems, most of those are cast in terms of Boolean variables, which find natural representations in terms of spin-1/2 systems acting as quantum bits. Thus most of those reduce to finding the ground state of some interacting spin-1/2 Hamiltonians. These universal simplicity in implementation keeps the quantum annealing format ahead of the circuit quantum computation in several important cases of combinatorial optimization problems.

2.5 Conclusion

In summary, it seems quantum annealing (or, for that matter, quantum computation at its present state) is not a panacea to all chronic computational handicaps. In particular, presence of strong disorder seems to limit its performance severely in general. But still use of quantum annealing can bring paradigm shifts in several areas of fundamental sciences by pushing the present limits on simulations to an extent which is almost impossible to parallel using classical computation at its present best. Of course question remains if a "proper" quantum annealer is foreseen in near future. It seems D-Wave incorporation has produced a quantum annealer that seems to perform certain tasks better than certain benchmarked classical computers (see [36,37], and articles by Albash et al., and Perdomo-Ortiz et al. in this issue). However, the superiority of the device over classical computers has not yet been established in general, and the "quantumness" of the machine is still debatable. Given the present status of technologies, a perfect scalable quantum annealer seems difficult to realize. But the question, is how much the imperfections affect the performance of the device? What kind of imperfections are fatal, and which are rather harmless? Questions of this sort are likely to keep the community busy in the coming days.

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