A Quantum Approach to Classical Statistical Mechanics

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We present a new approach to study the thermodynamic properties of $d$-dimensional classical systems by reducing the problem to the computation of ground state properties of a $d$-dimensional quantum model. This classical-to-quantum mapping allows us to deal with standard optimization methods, such as simulated and quantum annealing, on an equal basis. Consequently, we extend the quantum annealing method to simulate classical systems at finite temperatures. Using the adiabatic theorem of quantum mechanics, we derive the rates to assure convergence to the optimal thermodynamic state. For simulated and quantum annealing, we obtain the asymptotic rates of $T(t) \approx (pN)/(k_B \log t)$ and $\gamma(t) \approx (Nt)^{-\ell/N}$, for the temperature and magnetic field, respectively. Other annealing strategies, as well as their potential speed-up, are also discussed.

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An outstanding issue in combinatorial optimization is the classification of problems according to their computational complexity. Typically, one defines a cost function that needs to be minimized and the question is how the number of resources (e.g., time) to determine the minimum scales with the problem size $N$. Long time ago it has been recognized that certain physics problems can be cast in this language. For example, it has been shown that the computation of the ground state energy (or the partition function) of classical three-dimensional spin glasses belongs to the class of NP-complete problems \cite{1}, i.e. there is no known algorithm that can find the solution with polynomial (in $N$) resources. After all, the number of possible microscopic configurations of the system increases exponentially with the system size $N$ and, unless certain symmetries reduce the complexity, one has to search in an exponentially large state space. This simplification happens, for example, in the two-dimensional Ising spin glass \cite{2} (or any planar graph or lattice).

Simulated annealing (SA) \cite{3} and quantum annealing (QA) \cite{4} represent general algorithmic strategies to attack these optimization problems. The basic idea consists in finding the solution to the optimization problem as a limit of an effective physical process which uses additional variables or resources (e.g., time) to determine the minimum scales with the problem size $N$. In SA one introduces temperature $T$ as a tunable parameter: Initially the system is heated and next $T(t)$ is slowly decreased towards zero, eventually converging to the ground (lowest energy) state, whose energy equals the cost function. In QA, however, a time-dependent ad-hoc external magnetic field of magnitude $\gamma(t)$ is added to $H$, such that the total Hamiltonian can be interpreted as that of a quantum system. The (quantum) annealing process consists of slowly decreasing $\gamma(t)$ from a large value towards zero, while keeping $T = 0$. Since a quantum system in $d$ dimensions can be mapped onto another classical system in $d + 1$ \cite{5}, effectively in QA one is adding one extra space-dimension to the problem. In both strategies, the annealing procedure is essential to converge to the desired (ground) state, as it avoids getting stuck in local minima, using less resources than other optimization methods \cite{6}.

In this Letter, we propose new algorithms to study the thermodynamic properties of classical systems (including frustrated systems, such as spin glasses). The crux of the method consists of mapping the classical $d$-dimensional problem into a quantum problem of the same dimensionality, and then using techniques similar to those of QA to solve the latter. Our particular mapping allows us to unify the methods of SA and QA, and extend them to: i) study arbitrary classical models at $T > 0$ and ii) study new annealing schemes. From this classical-quantum mapping perspective, any annealing strategy differs by the choice of path in (quantum) Hamiltonian space. Computation of thermodynamic properties of the classical model amounts then to computation of ground state properties of the mapped quantum model. Our approach can be readily implemented on a classical computer (CC) by using existing stochastic methods, such as Green’s Function Monte Carlo \cite{6}, or by simulating the corresponding time-dependent Schrödinger equation. Since the proposed algorithms are based on a slow change of interactions in the quantum system, the rate at which these can be changed to assure convergence to the desired final state is determined by the adiabatic theorem \cite{7}. Remarkably, we will show that for the path corresponding to SA, the adiabatic condition yields to the result obtained by Geman and Geman on the rate of convergence to the optimal (ground) state of the classical system \cite{7}.

For simplicity, we study classical models defined on a lattice (or graph), where a variable $\sigma_j = \pm 1$ is defined on each site (vertex) $j$, and is related with the states of a physical spin $1/2$. Any spin configuration of the $2^N$ possible ones is denoted as $[\sigma] \equiv [\sigma_1, \ldots, \sigma_N]$, where $N$ is the total number of sites (or problem size). An energy functional $E[\sigma]$ (cost function) is defined on the lattice and its value depends on the state $[\sigma]$. For example, in the Ising model, $E[\sigma] = \sum_{ij} J_{ij} \sigma_i \sigma_j$, where two interacting spins $i$ and $j$ contribute $J_{ij}$ ($-J_{ij}$) to the en-
ergy if they are in the same (different) state(s). In the canonical ensemble, the expectation value of a thermodynamic variable $A$ at temperature $T$ is given by

$$ \langle A \rangle_T = \frac{1}{Z(T)} \sum_{\sigma} e^{-\beta E[\sigma]} A[\sigma], $$

(1)

where $Z(T) = \sum_{\sigma} e^{-\beta E[\sigma]}$ is the partition function and $\beta = 1/(k_B T)$, with $k_B$ the Boltzmann’s constant.

Any classical (finite-dimensional) spin model on a lattice can be associated with a quantum one, defined on the same lattice, by mapping every classical state $[\sigma]$ into a quantum state $|\sigma\rangle$. In this way, the energy functional maps into a Hamiltonian operator $H$. For spin-1/2 models, $H$ is given by mapping $\sigma_j^z \to \sigma_j^z$ in $E[\sigma]$, where $\sigma_j^z$ is the Pauli operator acting on the $j$th site. For example, $H = \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$ in the Ising model. The $N$-spin (unnormalized) quantum state $|\psi(T)\rangle = e^{-\beta H/2} \sum_{\sigma} |\sigma\rangle$ (i.e., the Gibbs state), satisfies

$$ \langle \hat{A} \rangle = \text{tr} [\rho \hat{A}] = \frac{\langle \psi(T) | \hat{A} | \psi(T) \rangle}{\langle \psi(T) | \psi(T) \rangle} \equiv \langle A \rangle_T, $$

(2)

where $\rho = e^{-\beta H}/Z(T)$. The operator $\hat{A}$ is determined by mapping the thermodynamic variable $A$, as described above. Then, $[\hat{A}, H] = 0$.

The state $|\psi(T)\rangle$ can be shown to be the ground state of a family of quantum Hamiltonians $H_q(T)$, which are defined on the same lattice. Each of these Hamiltonians can be connected through a similarity transformation to a possible transition matrix $M_q(T)$ of a Markovian process leading to the thermal distribution: $H_q(T) = 1 - e^{-\beta H/2} M_q(T) e^{\beta H/2}$. Interestingly, the interactions appearing in $H_q(T)$ are of comparable range to the interactions of the classical model. Therefore, a finite $T$ phase transition of a $d$-dimensional classical system can then be identified with a quantum phase transition of a $d$-dimensional quantum model. Thus, constructing a specific $H_q(T)$ and studying its ground state properties is of paramount importance as it will allow us to build different, yet more efficient algorithms to determine the thermodynamic properties of the classical system.

We obtain the simplest form of $H_q(T)$ in the following way. First, notice that the Pauli operator $\sigma_j^z$ (i.e., the spin-flip operator acting on the $j$th site) satisfies $\sigma_j^z e^{-\beta H/2} \sigma_j^z = e^{\beta H_j} e^{-\beta H/2}$, $\forall j \in \{1, N\}$. The Hamiltonian $H_j$ contains the terms in $H$ having the operator $\sigma_j^z$ (i.e., the terms in $H$ that anticommute with $\sigma_j^z$). Moreover, $\sigma_j^z \sum_{\sigma} |\sigma\rangle = \sum_{\sigma} |\sigma\rangle$, and $H_j(T)|\psi(T)\rangle = 0$, where $H_j(T) = \sigma_j^z - e^{\beta H_j}$. In the basis determined by the states $|\sigma\rangle$, the off-diagonal elements of $H_j(T)$ are non-negative, and the coefficients appearing in $|\psi(T)\rangle$ are all positive. The Perron-Frobenius theorem guarantees then that for $T > 0$, $|\psi(T)\rangle$ is the unique ground state of the irreducible quantum Hamiltonian $H_q(T) = -\chi \sum_j H_j^2(T)$. The coefficient $\chi = e^{-\beta p}$, with $p \approx \max_j |H_j| = O(1)$, is set for normalization purposes in order to satisfy $|H_q(T \to 0)| < \infty$. At this point, we would like to emphasize the simplicity of our particular mapping: The thermodynamic properties of any spin-1/2 classical system can be obtained by studying the ground state properties of a spin-1/2 quantum model, with classical interactions determined by $T$ and $H$ (i.e., the classical system), and an external (homogeneous) transverse field of magnitude $\chi$. Remarkably, this field generates quantum fluctuations that are in one-to-one correspondence with the classical fluctuations at temperature $T$. In particular, $H_q(T \to \infty) \approx (N - \sum_j \sigma_j^z)$, so its ground state has all spins aligned along the external field, i.e., $|\psi(T \to \infty)\rangle \approx \sum_{\sigma} |\sigma\rangle$. This quantum state can be identified with the completely mixed state in the classical model. In the limit of low $T$ we obtain $H_q(T \sim 0) \approx \chi \sum_j e^{\beta H_j}$, whose expectation value is minimized by the ground state(s) of the classical model, i.e., $|\psi(T \sim 0)\rangle$ is also a lowest energy state of $H$.

To illustrate these results, we consider the homogeneous one-dimensional Ising model $H = J \sum_{ij} \sigma_i^z \sigma_j^z$. In this case, $H_q(T) = \sigma_z - x^2 - xy(\sigma_x^{-1} \sigma_z + \sigma_x \sigma_z^{-1}) - \gamma^2 \frac{\sigma_x}{\sigma_z} - \gamma^2 \sigma_z^{-1}$, with $x = \cosh(\beta J)$, and $y = \sinh(\beta J)$. The Hamiltonian $H_q(T)$ denotes then a frustrated quantum Ising model, with next-nearest-neighbor interactions, and a transverse magnetic field of magnitude $\gamma$. Such a frustration forbids the existence of an ordered quantum phase unless $T \to 0$. This result is related to the non-existence of an ordered phase at finite temperature in the classical model.

Within our context, we can interpret the SA procedure as a (real time) quantum evolution where we start from the initial quantum state $|\psi(t \to \infty)\rangle \approx \sum_{\sigma} |\sigma\rangle$, and next we decrease the interaction parameter $T(t)$ (related to the temperature of the classical model) in $H_q(T)$. If such an evolution is performed adiabatically, we remain in the desired ground state $|\psi(T(t))\rangle$ at any time $t$. Therefore, the gap $\Delta(T)$ between the ground and first excited states of $H_q(T)$ plays an important role on the rate at which $T(t)$ must be decreased. This gap can be shown to satisfy $\Delta(T) \geq 2 \sqrt{\pi} e^{-\epsilon^2} N = \Delta(T)$. Such a lower bound can be determined using the inequalities in Ref. [12] and considering that $(N - H_q(T))$ is a strictly positive operator. It is based on the worst-case scenario (i.e., for the most general form of $H$), so it is expected to be improved depending on the nature of the interactions of the classical system, such as translational invariance. The rate of the evolution is then determined by the adiabatic condition

$$ \max_m \left| \frac{\langle \psi_m(T(t)) | \partial_T H_q(T) | \psi(T(t)) \rangle}{\Delta_m^2(T(t)) \sqrt{Z(T(t))}} \right| \partial_t T = \epsilon, \quad 0 \leq t \leq T, $$

(3)

where $\epsilon$ determines an upper bound to the probability of finding the system in any other (normalized) excited eigenstate $|\psi_m(T)\rangle$ of $H_q(T)$, $\Delta_m(T)$ is the energy gap between $|\psi_m(T)\rangle$ and $|\psi(T)\rangle$ (e.g., $\Delta_1(T) \equiv \Delta(T)$), and $T$ is the total time of the evolution. The lhs of Eq. (3) can be bounded above by $p N [2k_B T^2 \Delta(T)]^{-1} \partial_t T$. To see this, note that

$$ \partial_T H_q(T) |\psi(T)\rangle = [\partial_T (-\beta H/2), H_q(T)] |\psi(T)\rangle, $$

(4)
as \(-\beta H/2\) generates the translations of \(|\psi(T)\rangle\). Therefore,

\[
\frac{|\langle \psi_m(T)| H |\psi(T)\rangle|}{\Delta_m(T)} = \frac{|\langle \psi_m(T)| H |\psi(T)\rangle|}{(2k_BT^2)}, \quad (5)
\]

with \(|\langle \psi_m(T)| H |\psi(T)\rangle| \leq pN \sqrt{Z(T)}\). This upper bound is not necessarily tight. Equation (5) implies a resource requirement of \(T \approx O[1/c\Delta(T)]\) instead of \(T \approx O[1/c^2\Delta^2(T)]\), which is the common resource scaling associated with an adiabatic evolution. [Nevertheless, both scalings will yield to similar asymptotic behavior for \(T(t)\).] Integrating Eq. (5), replacing \(\min_m \Delta_m(T(t)) \) by \(\Delta(T(t))\), yields to

\[
T(t) \approx \frac{pN}{k_B \log(\alpha t + 1)}, \quad 0 < t \leq T, \quad (6)
\]

where \(\alpha\) decreases exponentially with the system size \(N\) and is proportional to \(\epsilon\), and \(T(\epsilon)\) is the temperature at which we want to study classical system. That is, if \(T(\epsilon)\) is decreased as given by Eq. (6), convergence to the desired state is guaranteed. In the limit \(T(T) \to 0\) and \(\log t \gg N \gg 1\), we obtain \(T(t) \approx (pN)/(k_B \log t)\) which agrees with the asymptotic convergence rate obtained in Ref. [3] for SA. Such an agreement relies on the fact that the energy gap of \(H_q(T)\) is also the energy gap of the transition matrix \(M_q(T)\), which is known to determine the mixing (or time required to reach thermal equilibrium) \(T_M \approx O(1/\Delta(T))\). That is, in the SA scheme one never departs from equilibrium if the temperature is decreased with the above convergence rate. Equivalently, in our context, the overlap between the adiabatically evolved quantum state and \(|\psi(T(t))\rangle\) is always close to 1. Note that Eq. (6) holds even if the interactions in \(H\) are of long-range nature.

QA has been proposed in Ref. [13] as an alternative method to reach the optimal (ground) state of a classical system with Ising-like interactions. Contrary to SA, the time-dependent quantum state in QA does not correspond, in general, to a thermal configuration of the original classical model. In this case, the quantum model Hamiltonian is given by \(H_q(\gamma) = H - \gamma \sum_j \sigma_j^z\), where \(\gamma\) is decreased from a very large value, corresponding to \(T \to \infty\), to \(\gamma \approx 0\), corresponding to \(T \approx 0\). If \(\gamma\) is slowly (adiabatically) changed, this method also allows us to reach the ground state of \(H\). Similar techniques have been proposed to study the complexity of solving NP-complete problems, such as 3-SAT, using a quantum computer (QC) [12]. Numerical and analytical results show that, for certain optimization problems, QA might enable a faster convergence rate to the optimal state than SA [13, 15, 16]. Faster convergence of QA could be attributed to a decrease in the probability of driving the classical system to a local minima, as its dimension is effectively increased by one. Nevertheless, it has also been observed that in some cases [17] QA performs similarly to SA. Note, however, that one could construct different Hamiltonian paths to approach the optimal state. Each path yields to a particular convergence rate that has to be determined on a case by case basis.

Using the classical-quantum mapping described above, the QA method can be extended to simulate classical statistical mechanics. To show this, we define a quantum Hamiltonian \(\hat{H}_q(\gamma) = \chi \sum_{ij} e^{\beta H} - \gamma \sum_j \sigma_j^z\), having \(|\psi(\gamma)\rangle\) and \(|\psi_m(\gamma)\rangle\) as ground and excited states. Here, \(\gamma\) is adiabatically decreased from a very large value towards \(\gamma \approx \chi\). In this way, the initial state \(\sum_{|\sigma|} |\sigma\rangle\) is transformed into the desired state \(|\psi(T)\rangle\). Notice that, from our viewpoint, QA differs from SA only by the choice of path used to reach the desired state. To successfully implement this annealing procedure, the rate at which \(\gamma\) must be decreased is determined by the adiabatic condition, i.e. by the gap \(\Delta(\gamma)\) between the ground and first excited states of \(\hat{H}_q(\gamma)\). This gap can be shown to satisfy \(\Delta(\gamma) \geq 2\sqrt{2\pi N e^{-N} (1 + c)^{-N}} \gamma = \Delta(\gamma)_0\), with \(c < \epsilon\). Like the SA case, and for the worst-case scenario, the adiabatic condition [13] yields to

\[
\gamma(t) \approx [(2N - 1)\bar{\alpha} t]^{-1/(2N - 1)}, \quad 0 < t \leq T, \quad (7)
\]

where \(\bar{\alpha}\) depends on \(N, \epsilon, \epsilon\), and \(\gamma(\epsilon) = \chi\) is determined by \(T\). In the limit \(\log t \gg N \gg 1\), and \(\gamma(\epsilon) \ll 1\), we obtain \(\gamma(t) \approx (2N \bar{\alpha} t)^{-1/(2N - 2)}\). If \(|\langle \psi_m(\gamma)| \partial_t \hat{H}_q(\gamma) |\psi(\gamma)\rangle| \leq x \Delta_m(\gamma)\), with \(\Delta_m(\gamma)\) the corresponding energy gap and \(x = O(N^2)\), the coefficient \(2N\) in Eq. (7) can then be replaced by \(N\). In this manner, the convergence rate is in agreement with the result obtained in Ref. [16]. Note, however, that this annealing schedule does not provide an advantage with respect to SA as \(\gamma\) must be decreased to \(\gamma(T) = \chi\), which is exponentially small in \(1/T\).

The QA procedure to simulate \(T > 0\) can be directly implemented on a QC [18]. If the path-integral Monte Carlo method is chosen to simulate a \(d = 1\) Ising-like model with nearest-neighbor interactions, \(\hat{H}_q(\gamma)\) has to be mapped onto the 2-dimensional classical model, with energy functional

\[
\tilde{E}[\sigma] = \tilde{\beta} \sum_{i,j} \tilde{J}_{ij}(\beta) \sigma_{i\sigma} \sigma_{j\bar{\sigma}} + \xi(\beta, t) \sum_{k=1}^{L} \sum_{i=0}^{\bar{L}} \sigma_{ik} \sigma_{i(k+1)} \quad (8)
\]

Here, \([\sigma] = [\sigma_{11}, \sigma_{21}, \ldots, \sigma_{NL}]\) is one of the \(2^{NL+L}\) possible spin configurations, and \(\sigma_{ik} = \pm 1\). The parameter \(L\) denotes the number of copies of the system in the extra dimension (i.e., the Trotter discretization) and satisfies \(L \gg 1\). The coupling constants \(\tilde{J}_{ij}(\beta)\) are defined via \(\tilde{\chi} \sum_{ij} e^{\beta H} \equiv \Lambda(\beta) + \sum_{ij} \tilde{J}_{ij}(\beta) \sigma^z_i \sigma^z_j\), with \(\tilde{J}_{ij}(\beta \to 0) \approx 0\). The coefficient \(\tilde{\beta}\) is given by the effective temperature of the quantum system and is not related with the temperature at which the classical system is studied. Therefore, \(\tilde{\beta} \gg 1\) and \(\tilde{\beta}/L = \delta\tau\), with \(\delta\tau\) being the time-slice of the discretization. The (ferromagnetic) coupling between two adjacent copies is determined by \(\xi(t) = \log\cosh(\tilde{\beta}\chi\gamma(t)/L)/2\), and its magnitude increases as the transverse field \(\gamma(t)\) decreases to \(\gamma(T) = \chi\), determined by \(T\). In order to simulate more general classical systems at finite temperatures, the interactions appearing in Eq. (8) must be modified accordingly.

Note that the classical-quantum mapping can be extended and used to study any (finite-dimensional) classical system other than Ising-like models. In particular, it can be extended
to simulate $s$-spin classical systems ($s > 1/2$), where a variable $\sigma_j = [-s, -s + 1, \ldots, s - 1, s]$ is defined on each site $j$. In the case of QA, the ground state of $H_\gamma^q(\gamma) = \chi \sum_j e^{\beta H_j} - \gamma \sum_j X_j$ will determine the statistical properties of the classical model when $\gamma \to \chi$. The operators $X_j \in \mathfrak{su}(2s + 1)_j$ satisfy $[X_j, S^z_j] = 0$, $\forall i \neq j$, and $X_j S^z_j = -S^z_j X_j$, with $X_j^2 = \mathbb{I}$. Here, $S^z_j \in \mathfrak{su}(2)$ is the angular momentum operator along the $z$-axis and determines $H_j$. In matrix representation, $X$ has 1’s in the anti-diagonal and 0’s otherwise. For example, in the $s = 1$ three-state Potts model $[19]$, $E[\sigma] = J \sum_j \delta(\sigma_j, \sigma_{j+1})$ and $H = J/2\sum_j [S^z_j S^z_{j+1} + 1 + S^z_j S^z_{j+1}] - 2[(S^z_j)^2 + (S^z_{j+1})^2]/2$. Therefore, $H_j = J/2[S^z_j S^z_{j+1} + 1 + S^z_j S^z_{j+1}]$ and $X_j = 1 - (S^z_j)^2 + [(S^z_j)^2 + (S^z_{j+1})^2]/2$, defining the corresponding $H_\gamma^q(\gamma)$.

The annealing schedule is again determined by adiabatically changing $\gamma(t)$ from a large value, where the initial state of the system is $\sum_{[\sigma]} [\sigma]$), to $\gamma(T) = \chi = e^{-\beta \gamma}$, where the final state of the system is $e^{-\beta H/2} \sum_{[\sigma]} [\sigma]$. It is important to stress that one can easily implement this extended QA (EQA) procedure by using current numerical methods. Since our analysis has only focused on the worst-case scenario, we would expect that for certain problems EQA should outperform SA [13]. Moreover, one can always design other annealing procedures than the ones we have described. This can be done by constructing other quantum Hamiltonians having $|\psi(T)\rangle$ as their ground state, and by introducing an extra interaction that is slowly changed to converge to the desired state. Depending on the path considered, it is expected a different behavior for the way that the relevant energy gap closes, and a different convergence rate as determined by the adiabatic condition.

So far, we have considered that the lower bound in the gap is exponentially small in $\beta N$, for SA, or $N \log \gamma$, for QA. One may wonder what the convergence rate for $T(t)$ or $\gamma(t)$ is, when the gap can be bounded below by $(\beta N)^{-1/4}$ or $(N \log \gamma)^{-1/4}$, with $q \geq 0$ independent of $N$ and $\beta$. In this case, integration of Eq. [1] yields to a convergence rate for SA of $T(t) \approx O(t^{1/(q+1)})$, with $a$ a constant that depends on $N$ and $\epsilon$. This is a much faster convergence rate than the one obtained in Eq. [4].

In this Letter, we have shown how to simulate the thermodynamic properties of an arbitrary classical model in $d$ dimensions by studying the ground state properties of a $d$ dimensional quantum system. This was achieved by an exact classical-quantum mapping. We have used the adiabatic theorem of quantum mechanics to analyze the convergence rate and resources required to reach the corresponding ground state. Our approach provides a unifying framework to address on an equal footing the well-known optimization methods of simulated and quantum annealing. These annealing procedures can be understood as two different evolution paths of the quantum system. It is remarkable, that the annealing rates obtained by using the adiabatic condition are in agreement with previous known results [8] [14], which were obtained in the context of stochastic approaches such as path-integral or Green's function Monte Carlo. It is expected, however, that a QC will require less resources (e.g., quadratic speed-up) than a CC to solve these optimization problems. This issue will be addressed elsewhere.

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