Optimization and thermodynamics of classical problems from a quantum perspective

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Abstract. We present two approaches to study the thermodynamic properties of $d$-dimensional classical systems in equilibrium. In the first approach we reduce this problem to the computation of the ground state properties of a $d$-dimensional quantum model. This classical-to-quantum mapping allows us to extend the scope of standard optimization methods by unifying them under a general framework. Particularly, we extend the quantum annealing method to study classical systems at finite temperatures. We derive the rates to assure convergence to the optimal thermodynamic state using the adiabatic theorem of quantum mechanics. In the second approach we present a quantum algorithm that performs numerical integration and computes, for example, the partition function of the system under study. We show that this quantum algorithm provides a quadratic speed-up with respect to the classical algorithm that samples with the uniform distribution and computes physical quantities of interest. Other quantum strategies, as well as their potential speed-up, are also discussed.

1. Introduction
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 and space) 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 computing the ground state energy (or the partition function) of a classical three-dimensional spin glass is an NP-hard problem [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 one has to search in this exponentially large configuration space to find the solution. In a few cases, however, this complexity can be reduced by using adequate methods that allow one to solve the problem with significantly less resources. This simplification occurs, for example, in the two-dimensional Ising spin glass [1].

Simulated annealing (SA) [2] and quantum annealing (QA) [3, 4] represent general algorithmic strategies to attack these optimization problems. Adiabatic optimization [5] and QA are essentially the same methods. 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 dimensions, and where the cost function is identified with a Hamiltonian $H$ of a classical physical system. In SA a temperature $T$ is introduced 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 \textit{ad-hoc} transverse magnetic field, $\gamma(t)$, is added to $H$, such
that the total Hamiltonian can be interpreted as that of a quantum system. The QA process consists of slowly decreasing $\gamma(t)$ from a large value to zero, while keeping $T = 0$. Since a quantum system in $d$ dimensions can be mapped onto another classical system in $d + 1$ [6], the QA procedure adds one extra space-dimension. In both strategies, the annealing procedure is meant to avoid getting stuck in local minima, potentially converging to the desired (ground) state [7].

In this paper, we propose two quantum approaches to study the thermodynamic properties of classical systems (including frustrated systems, such as spin glasses). The crux of the first approach consists of mapping the classical $d$-dimensional problem into a quantum problem of the same dimensionality, and use techniques similar to those of QA for solving the latter [8]. Our particular mapping allows us to unify the methods of SA and QA, and extend them to: i) study arbitrary classical models at $T > 0$, ii) study new annealing schemes. From this new perspective, any annealing strategy differs by the choice of path in (quantum) Hamiltonian space. The computation of thermodynamic properties of the classical model amounts then to computation of ground state properties of the mapped quantum model. 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 [9]. 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 [10]. Our first approach can be readily implemented on a classical computer (CC) by using existent stochastic methods, such as Green’s Function Monte Carlo [11], or by simulating the corresponding time-dependent Schrödinger equation, or by using renormalization group (DMRG) techniques [12].

In the second approach we develop a quantum (computing) algorithm that can be interpreted as the quantum version of the classical algorithm that picks any state configuration at random (i.e. it samples with the uniform distribution), computes its Boltzmann weight, and estimates the partition function or any other observable property by integration. We show that this quantum method provides a speed-up as it exploits quantum coherence using subroutines like amplitude amplification and phase estimation [13]. While in this paper we only give a brief description of how this method works, a detailed explanation will be given in reference [14].

2. Classical-to-Quantum Mapping
For simplicity, we study classical models on a lattice (or graph), where a variable $\sigma_j = \pm 1$ is defined on each site (vertex) $j$, and represents a physical spin-$1/2$. A given spin configuration of the $D = 2^N$ possible ones is denoted as $[\sigma] \equiv [\sigma_1, \ldots, \sigma_N]$, where $N$ is the total number of sites. An energy functional $E[\sigma]$ (cost functional) 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 energy if they are in the same (different) state(s). In the canonical ensemble, the expectation value of a thermodynamic variable $A$ is given by

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

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

Any classical (finite-dimensional) spin model on a lattice can be associated to a quantum model, 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 the eigenvalues of the Hamiltonian operator $H$. For spin-$1/2$ models, $H$ is given by mapping $\sigma_j \rightarrow \sigma_j^z$ 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
|ψ(T)⟩ = e^{-βH/2} \sum_\sigma |\sigma⟩ \langle \sigma|, satisfies

⟨\hat{A}⟩ = \text{tr} [\rho \hat{A}] = \frac{⟨\psi(T)|\hat{A}|\psi(T)⟩}{⟨\psi(T)|\psi(T)⟩} \equiv ⟨A⟩_T,

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

The state |ψ(T)⟩ can be shown to be the ground state of a family of quantum Hamiltonians H_q(T) [15], which are defined on the same lattice. Each of these H_q(T) 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^{βH/2} M_q(T) e^{-βH/2}. Interestingly, the interactions appearing in H_q(T) and H are of comparable range. 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 properties of the classical system at any finite T.

The simplest form of H_q(T) is obtained in the following way. We first note that the Pauli operator \sigma^z_j satisfies \sigma^z_j e^{-βH/2} \sigma^z_j = e^{βH_j} e^{-βH/2}, \forall j \in [1, N]. The Hamiltonian H_j only includes the terms in H that contain the operator \sigma^z_j (i.e., the terms in H that anticommute with \sigma^z_j). Moreover, \sigma^z_j \sum_\sigma |\sigma⟩ \langle \sigma| = \sum_\sigma |\sigma⟩ \langle \sigma|, and H^1_q(T)|ψ(T)⟩ = 0, where H^1_q(T) = \sigma^z_j - e^{βH_j}. In the basis of states |\sigma⟩, the off-diagonal elements of H^1_q(T) are non-negative, and the coefficients appearing in |ψ(T)⟩ are all positive. The Perron-Frobenius theorem [16] guarantees then that for T > 0, |ψ(T)⟩ is the unique ground state of the irreducible quantum Hamiltonian H_q(T) = -\chi \sum_j H^1_q(T). The scale of H_q(T) is chosen as χ = e^{-βp}, with p \approx \max_j |H_j| = O(1), in order to satisfy |H_q(T \to 0)| < ∞. We emphasize the simplicity of our particular construction: 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 ∞) \approx (N - \sum_j \sigma^z_j), so its ground state has all spins aligned along the external field, i.e. |ψ(T \to ∞)⟩ \approx \sum_\sigma |\sigma⟩ \langle \sigma|. This quantum state can be identified with the completely mixed state (uniform Boltzmann weights) of the classical model for T → ∞. In the low-T limit, we obtain H_q(T \to 0) \approx \chi \sum_j e^{βH_j}, whose expectation value is minimized by the ground state(s) of the classical model, i.e. |ψ(T \to 0)⟩ is also a lowest energy state of H.

To illustrate these results, we consider the homogeneous one-dimensional Ising model H = J \sum_{i,j} \sigma^z_i \sigma^z_j. In this case, H^1_q(T) = \sigma^z_j - x^2 - xy(\sigma^z_i \sigma^z_j + \sigma^z_j \sigma^z_i - 1) - y^2 \sigma^z_i \sigma^z_j, with x = \cosh(βJ), and y = \sinh(βJ). The Hamiltonian H_q(T) denotes then a frustrated quantum Ising model, with next-nearest-neighbor interactions, and a transverse magnetic field of magnitude \chi. Due to the one-dimensional character of H_q(T) and the finite range of its interactions, an ordered phase can only appear at T = 0.

3. Unifying framework for different optimization strategies:

Rates of convergence and the adiabatic theorem of Quantum Mechanics

In this context, SA corresponds to a (real-time) quantum evolution with initial quantum state |ψ(T \to ∞)⟩ \approx \sum_\sigma |\sigma⟩. The system evolves by changing continuously the interaction parameter T(t) (related to the temperature of the classical model) in H_q(T). If the evolution is adiabatic, the system remains in the ground state, |ψ(T(t))⟩, of the snapshot Hamiltonian, H_q(T(t)), at any time t. Therefore, the gap Δ(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 Δ(T) ≥ 2\sqrt{2\pi N e^{-(βp+1)} N} = \bar{Δ}(T).
Such a lower bound can be determined by using the inequalities in reference [17] and considering that \( \tilde{S} = (N - H_{q}(T))^{N} \) is a strictly positive (symmetric) operator. In fact, every matrix element of \( \tilde{S} \) satisfies \( |\tilde{S}_{ij}| \geq N!^{\chi N} \approx N!e^{-\beta pN} \). This lower bound can be obtained by considering the least probable physical process of flipping all spins at once. Then [17], \( |\lambda| \leq \frac{K-1}{\lambda_{mix}} N^N \), with \( |\lambda| \) the norm of the second largest eigenvalue of \( \tilde{S} \), \( K = \max_{ijkl} \sqrt{\frac{\tilde{S}_{ij} \tilde{S}_{kl}}{\tilde{S}_{ik} \tilde{S}_{lj}}} \) and \( N^N \) corresponds to the largest eigenvalue of \( \tilde{S} \).

Since \( \min_{ij} \tilde{S}_{ij} \geq \frac{\sqrt{2\pi N}N^{N-1}e^{-(\beta p+1)N}}{\sqrt{2\pi N}} \) (i.e., Stirling’s approximation) and \( \max_{ij} \tilde{S}_{ij} < N^N \), we have \( K < \frac{\sqrt{2\pi N}N^{N-1}e^{-(\beta p+1)N}}{\sqrt{2\pi N}} \). Then, the spectral gap \( \Delta_{m} \) of \( \tilde{S} \) satisfies \( \Delta_{m} = N^N - E_{1}N \geq 2N^{N-1}e^{-(\beta p+1)N}\sqrt{2\pi N} \), where we replaced \( |\lambda| \) by \( E_{1}N \), with \( E_{1} \) the second largest eigenvalue of \( N - H_{q}(T) \). Finally, since \( N^{N}(N - E_{1}) = N^{N}\Delta(T) \geq N^{N} - E_{1}N \), we arrive to the desired result \( \Delta(T) \geq N^{N}e^{-(\beta p+1)N} = \Delta(T) \). Note that this result is actually 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.

The rate of the evolution is then determined by the adiabatic condition [9]

\[
\max_{m} \left| \frac{\langle \psi_{m}(T(t)) \rangle}{\partial_{t}H_{q}(T)\langle \psi(T(t)) \rangle} \right| = \epsilon, \quad 0 \leq t \leq T, \tag{3}
\]

where \( \epsilon \) determines an upper bound to the probability of finding the system in any other (normalized) excited eigenstate \( \langle \psi_{m}(T) \rangle \) of \( H_{q}(T) \), \( \Delta_{m}(T) \) is the energy gap between \( \langle \psi_{m}(T) \rangle \) and \( \langle \psi(T) \rangle \) (e.g., \( \Delta_{1}(T) \equiv \Delta(T) \)), and \( T \) is the total time of the evolution. The lhs of equation (3) can be bounded above by \( pN[2k_B T^2\Delta(T)]^{-1} \partial_{t}T \). To see this, note that

\[
\partial_{t}H_{q}(T)\langle \psi(T) \rangle \equiv \partial_{t}(-\beta H/2), \quad H_{q}(T)\langle \psi(T) \rangle, \tag{4}
\]

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

\[
\frac{\left| \langle \psi_{m}(T) \rangle / \partial_{t}H_{q}(T)\langle \psi(T) \rangle \right|}{\Delta_{m}(T)} = \frac{\left| \langle \psi_{m}(T) \rangle H\langle \psi(T) \rangle \right|}{(2k_B T^2)}, \tag{5}
\]

with \( \left| \langle \psi_{m}(T) \rangle H\langle \psi(T) \rangle \right| \leq pN\sqrt{Z(T)} \). This upper bound is not necessarily tight. Equation (5) implies a resource requirement of \( T \approx O[1/\epsilon \Delta(T)] \) instead of \( T \approx O[1/\epsilon \Delta^{2}(T)] \), which is the common resource scaling associated with an adiabatic evolution. [Nevertheless, both scalings will yield to similar asymptotic behavior for \( T(t) \).] Integrating equation (3), replacing \( \min_{m}[\Delta_{m}(T(t))] \) by \( \Delta(T(t)) \), yields to

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

where \( \alpha \propto \epsilon \) decreases exponentially with \( N \), and \( T(t) \) is the desired temperature for the classical system. That is, if \( T \) decreases according to equation (6), the 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 reference [10] for SA. Such an agreement results from the fact that the energy gap of \( H_{q}(T) \) is also the gap \( \Delta(T) \) of \( M_{q}(T) \). This gap determines the mixing time \( T_{mix} \), which is the time required to get sufficiently close to thermal equilibrium \( \bar{P}_{eq}(T) = M_{q}(T)\bar{P}_{eq}(T) \) with \( \bar{P}_{eq}(T) = (Z(T))^{-1}(e^{-\beta E_{1}}, \cdots, e^{-\beta E_{D}}) \). To show this, we define the probability distribution of the classical system at time \( t, \bar{P}_{t} \), satisfying \( \bar{P}_{t} = [M_{q}(T)]^{M} \bar{P}_{t=0}, \) where \( t = M \tau \) and \( \tau \) is a time step, such that \( \bar{P}_{\tau \to \infty} = \bar{P}_{eq} \). Since the largest eigenvalue of \( M_{q}(T) \) is 1, the time it takes for \( \bar{P}_{t} \) to differ from \( \bar{P}_{eq} \) by \( 1/(\epsilon t) \) is \( T_{mix} \approx O[1/\epsilon \Delta(T)] \). This in turn implies a similar condition for the convergence rate of \( T(t) \), determined by equation (6), such that the classical system remains close to equilibrium along the SA process. Equivalently, in our context, the overlap between the adiabatically evolved quantum state and \( \langle \psi(T(t)) \rangle \) is always close to 1. Note that equation (6) holds even if the interactions in \( H \) are of long-range nature.
QA has been proposed in reference [3] 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 $H$. Numerical and analytical results show that, for certain optimization problems, QA might enable a faster convergence rate to the optimal state than SA [3, 18, 19]. Faster convergence of QA could be attributed to a decrease in the probability of 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 QA performs similarly to SA [20].

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 systems at any finite $T$. To show this, we define a quantum Hamiltonian $H_q(\gamma) = \chi \sum_j e^{\beta H_j} - \gamma \sum_j \sigma_j^z$, having $|\psi(\gamma)\rangle$ and $|\psi_m(\gamma)\rangle$ as ground and excited states. Here, $\gamma$ is adiabatically decreased from a very large value to $\gamma \approx \chi$. 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 of change of $\gamma$ is determined from the adiabatic condition, i.e. by the gap $\Delta(\gamma)$ between the ground and first excited states of $H_q(\gamma)$. Performing a similar analysis as above, this gap can be shown to satisfy $\Delta(\gamma) \approx 2\sqrt{2\pi N} e^{-N}(1 + c)^{-N} \gamma^N = \Delta(\gamma)$ [17], with $c < 1$. For the worst-case scenario, the adiabatic condition [9] yields to

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

where $\bar{\alpha}$ depends on $N$, $c$, and $e$, and $\gamma(T) = \chi$ is determined by $T$. In the limit $\log t \gg N \gg 1$, and $\gamma(T) \ll 1$, we obtain $\gamma(t) \approx (2N\bar{\alpha} t)^{-1/2N}$. If $|\langle \psi_m(\gamma) | \partial_\gamma H_q(\gamma) | \psi(\gamma) \rangle | \leq x \Delta_m(\gamma)$, with $\Delta_m(\gamma)$ the corresponding energy gap and $x \approx O(N^2)$, the coefficient $2N$ in equation (7) can then be replaced by $N$. In this manner, the convergence rate is in agreement with the result obtained in reference [19]. 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 CC. If the path-integral Monte Carlo method is chosen to simulate a $d = 1$ Ising-like model with nearest-neighbor interactions, $H_q(\gamma)$ has to be mapped onto the 2-dimensional classical model, with energy functional

$$\bar{E}[\sigma] = \frac{\beta}{L} \sum_{k=1}^L \sum_{ij} \tilde{J}_{ij}(\beta) \sigma_{ik} \sigma_{jk} + \xi(\beta, t) \sum_{k=1}^L \sum_{i=0}^N \sigma_{ik} \sigma_{i(k+1)}.$$  

Here, $[\sigma] = [\sigma_{11}, \sigma_{21}, \cdots, \sigma_{NL}]$ is one of the $2^{N+L}$ 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 $\chi \sum_j e^{\beta H_j} = \Lambda(\beta) + \sum_{ij} \tilde{J}_{ij}(\beta) \sigma_i^z \sigma_j^z$, 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 to the $T$ at which the classical system is studied. Therefore, $\tilde{\beta} \gg 1$ and $\tilde{\beta}/L$ is the time-slice of the discretization. The (ferromagnetic) coupling between two adjacent copies

\footnote{It is important to emphasize that, as is expected for the simulation of classical systems, the simulations presented in this work do not suffer from the so-called sign(phase)-problem since all the coefficients in the expansion of the exact ground state, in terms of the standard basis, are real and positive. This implies the possibility of finding an irreducible quantum Hamiltonian $H_q$ with non-negative off-diagonal elements such that the quantum state is the highest-energy state of $H_q$. Nevertheless, many optimization problems (e.g., the $d = 3$ Ising glass) are known to be NP-hard. This implies that the sign(phase)-problem may be a sufficient but not necessary condition for a problem to be NP-hard.}
is determined by $\xi(t) = \log[\cosh(\beta \chi(t)/L)]/2$, 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 $T$, the interactions appearing in equation (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 easily extended to simulate any classical spin system with $s > 1/2$. In the case of QA, the ground state of $\hat{H}_q(\gamma) = \chi \sum_j e^{\beta H_j} - \gamma \sum_j X_j$ will determine the statistical properties of the classical model when $\gamma \to \chi$. The operators $X_j \in \text{su}(2s + 1)_j$ satisfy $[X_j, S^j_z] = 0$, $\forall i \neq j$, and $X_j S^j_z = -S^j_z X_j$, with $X_j^2 = \mathbb{I}$. Here, $S^j_z \in \text{su}(2)_j$ 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 [21], $E[\sigma] = J \sum_j H_j$ and $H = J \sum_j [\mathbb{I} + S^j_z S^{j+1}_z (1 + 3 S^j_z S^{j+1}_z)/2 - (S^j_z)^2 - (S^{j+1}_z)^2]$. Therefore, $H_j = J/2 [S^j_z S^{j+1}_z + S^{j+1}_z S^j_z] + 1 - (S^j_z)^2 + [(S^j_z)^2 + (S^{j+1}_z)^2]/2$, defining the corresponding $H^e_{s=1}(\gamma)$. The annealing schedule is again determined by changing $\gamma(t)$ adiabatically, from the initial state $\sum_{[\sigma]} \langle [\sigma]|\psi(0)\rangle$, to $\gamma(T) = \chi = e^{-\beta P}$. The final state of the system is $e^{-\beta H/2} \sum_{[\sigma]} \langle [\sigma]|\psi(T)\rangle$.

We stress that this extended QA (EQA) procedure can be easily implemented by using current numerical methods. Our analysis has focused on the worst-case scenario (i.e., exponential bounds on the gap). Since EQA has more flexibility in the choice of Hamiltonian path, we would expect that EQA should outperform SA [3, 20]. Moreover, many other annealing procedures can be designed by exploiting the classical–quantum mapping. 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. The relevant energy gap closes in different ways depending on the path that is considered, leading to different convergence rates determined by the adiabatic condition. Note that equations (6) and (7) have been obtained by the conditions in reference [9] and one could argue that these are not strictly rigorous. Nevertheless, if a rigorous condition can be found by considering higher powers of the energy gap [22], the asymptotic behavior of equations (6) and (7) still persists.

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 $(\beta N)^{-1/q}$ or $(N \log \gamma)^{-1/q}$, with $q \geq 0$ independent of $N$ and $\beta$. In this case, integration of equation (3) yields to a convergence rate for SA of $T(t) \approx \mathcal{O}(\alpha t^{1/(q+1)})$, with $\alpha$ a constant that depends on $N$ and $\epsilon$. This is a much faster convergence rate than the one obtained in equation (6).

4. Quantum algorithms for numerical integration with no importance-sampling

When one is interested in computing functions like the partition function using numerical integration, several methods can be used. Maybe the simplest one realizes integration by sampling states randomly, inferring the value of the integral after certain number of samplings. For example, when computing the partition function $Z(T)$ for a state space of dimension $2^N$ (i.e. $N$ spins 1/2) after $M$ samplings, the partition function is estimated as

$$Z(T) \to \hat{Z}(T) = \frac{2^N}{M} \sum_{n=1}^{M} e^{-\beta E[\sigma_n]} \tag{9}$$

with $\sigma_n$ the state sampled in the $n$th step. Note that $\hat{Z}(T)$ is just the average of the stochastic function $X(E) = 2^N e^{-\beta E}$. A good measure for the absolute error in the estimation after $M$ samplings is given by

$$\frac{2^N \sqrt{\langle \epsilon^{-2\beta E} \rangle - \langle \epsilon^{-\beta E} \rangle^2}}{\sqrt{M}}, \tag{10}$$

where the expectation values are now taken over the probability distribution inferred in $X(E)$ by the uniform sampling of states. If $\beta \ll 1$ the probability that $X(E) \approx 2^N$ is close to one, so the uncertainty approaches to zero in these cases and only a small $M$ is necessary.
Clearly, this method could become very inefficient at low temperatures where only a small region of the state space becomes important. In the latter case, sampling with a uniform distribution returns those “relevant” states with low probabilities. Nevertheless, for the sake of simplicity, here we focus on the quantum version of this integration method to show that speed-ups are attainable, and those cases where importance sampling may reduce the complexity will be discussed in reference [14].

The quantum algorithm that simulates the above integration method begins with the equal superposition state \( \frac{1}{\sqrt{2^n}} \sum_{|\sigma\rangle} |\sigma\rangle \), where we use the index \( S \) to denote the “system”. This is equivalent to begin with the uniform distribution in the classical case. We then add an extra qubit (spin-1/2), called ancilla \( a \), initialized in the state \( |0\rangle_a \). This ancilla will be rotated to the state \( |1\rangle_a \) with probability \( 1 - p(\sigma) = 1 - e^{-\beta E(\sigma)} \), controlled in the state \( |\sigma\rangle \). To do this, only a single call to a reversible “classical” box that computes \( p(\sigma) \) (with certain bit precision) when the input is \( |\sigma\rangle \) is necessary. The unitary that rotates \( a \) is determined then by \( R = e^{-i \arccos(\sqrt{p(\sigma)})} \sigma_\pm^a \). Note that we assumed \( E(\sigma) \leq 0 \), \( \forall \ |\sigma\rangle \) to satisfy \( p(\sigma) \leq 1 \). This can be done by adding an irrelevant constant to the energy functional of the classical system without changing the thermodynamic properties. The state so prepared, with only one computation of \( p(\sigma) \) (which corresponds to sample only once), is

\[
|\phi(T)\rangle = U(T)|0\rangle_S|0\rangle_a = \frac{1}{\sqrt{2^N}} \sum_{|\sigma\rangle} |\sigma\rangle_S (\sqrt{p(\sigma)}|0\rangle_a + \sqrt{1 - p(\sigma)}|1\rangle_a),
\]

with \( U(T) \) the unitary operator that prepared \( |\phi(T)\rangle \) out of some initial, boot-up, state \( |0\rangle_S|0\rangle_a \).

Interestingly, if the ancilla were measured in the computational basis and projected onto \( |0\rangle_a \), the state \( |\psi(T)\rangle \) of the previous sections would be prepared with almost no cost. However, this is unlikely as the probability of such event (that is, the probability of projecting the state of the ancilla onto \( |0\rangle_a \) after a measurement) may be exponentially small.

Several strategies could be followed to compute \( Z(T) \). A possible one would be to compute the expectation of the projector \( |0\rangle_a\langle 0| \equiv (\mathbb{I} - \sigma_\pm^a)/2 \), that is

\[
o = \langle \phi(T)| \left( \frac{\mathbb{I} - \sigma_\pm^a}{2} \right) |\phi(T)\rangle = \frac{Z(T)}{2^N}.
\]

Interestingly, if \( 1/\sqrt{M} \) is the precision to be returned by a quantum algorithm that computes \( o \), only \( \sqrt{M} \) calls to the unitary \( U(T) \) are necessary [13]. In this case, the overall precision in the estimation of \( Z(T) \) is given by \( 2^N/\sqrt{M} \), which is comparable to the one in equation (10).

In more detail, our quantum algorithm computes \( \phi' = \langle 0|\sigma_\pm^a U(T)|0\rangle_S|0\rangle_a \) at a precision of order \( 1/\sqrt{M} \). If \( \phi \) is defined such that \( \cos(\phi) = \phi' \), that is \( 2\phi \) is the angle between the states \( |0\rangle_S|0\rangle_a \) and \( U(T)|\sigma_\pm^a U(T)|0\rangle_S|0\rangle_a \) in the Bloch-sphere (spin-1/2) representation, one can build a unitary operator \( U \) by composing two reflections onto those states having \( \pm \phi \) as eigenphases. Therefore, one can use well known phase estimation algorithms to obtain \( \phi \) and thus \( \phi' \) [13]. Remarkably, these phase estimation algorithms return a precision of order \( 1/\sqrt{M} \) in \( \phi \) with only \( \sqrt{M} \) uses of \( U(T)|\sigma_\pm^a U(T) \). Moreover, as explained before, each action of \( U(T) \) or \( U(T) \) requires a single call to the “classical” box that computes \( p(\sigma) \). At the end, only \( \sqrt{M} \) calls are necessary which is a quadratic improvement over the \( M \) samplings necessary in the classical setting to achieve a precision of similar order.

5. Conclusions
In this paper, we started by showing 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 obtained from 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 first 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 [10, 19], which were obtained in the context of stochastic approaches such as path-integral or Green’s function Monte Carlo.

In the second approach we have developed a quantum algorithm that can be understood as the quantum analogue of the classical algorithm that samples with the uniform distribution. We have shown that by exploiting quantum coherence and using well known methods like phase estimation, a quadratic increase in precision of partition function estimation (or a quadratic decrease in resources) can be achieved in the quantum case. These results will be generalized elsewhere [14].

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