

A Review of Quantum Adiabatic Optimisation

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The quantum adiabatic algorithm involves the translation of a combinatorial optimisation problem into a quantum mechanical variational problem. Initially, one identifies a quantum mechanical system with a Hamiltonian operator \mathcal{H} whose expectation values $\langle \mathcal{H} \rangle_\psi := \langle \psi, \mathcal{H} \psi \rangle$ can be isomorphically mapped via a functor ϕ into the objective function f of the combinatorial optimisation problem. This mapping $\phi : \langle \mathcal{H} \rangle_\psi \mapsto f$ equates the task extremising cost function to finding the energy of the ground state in the quantum mechanical system. The insight of utilizing concepts originating from statistical physics for the resolution of combinatorial optimisation problems can be discerned in the seminal works of Metropolis *et al.* [14], as well as in the contributions of Kirkpatrick *et al.* [12]. A comparable application of such ideas from a Darwinian perspective can be attributed to Dunham *et al.* [8]. For a contemporary overview of adiabatic quantum computation, the interested reader is referred to the comprehensive review provided in references [2, 7].

To commence, let us evoke the rigorous mathematical definition of a combinatorial optimization problem [21].

Definition 1. Let us recall that an N -dimensional combinatorial optimisation problem is an ordered triple $\mathcal{P} := \langle \Omega, \mathcal{S}, f \rangle$, where $\Omega \subseteq \mathbb{Z}^N$ is a non-empty discrete set with finite cardinality, referred to as the *solution space*, $\mathcal{S} \subset \Omega$ is a proper-subset the members of which are called *feasible solutions*, and $f : \Omega \rightarrow \mathbb{R}$ is the ob-

*jective function*¹. A necessary and sufficient condition in order for the optimisation problem \mathcal{P} to possess a solution $\omega \in \mathcal{S}$ is that either $f(\omega) = \min_{\tau \in \mathcal{S}} f(\tau)$ or $f(\omega) = \max_{\tau \in \mathcal{S}} f(\tau)$. In the former scenario, \mathcal{P} is referred to as a minimisation problem, whereas in the latter, \mathcal{P} is termed a maximisation problem.

A prominent example illustrating the map between combinatorial optimisation problems and quantum mechanical systems is the dictionary of the Traveling Salesman Problem (TSP) into the Ising spin-glass model within quantum statistical physics. For the sake of completeness, we review the rigorous mathematical definition of the Ising model. A complete discussion can be found in ref. [10].

Definition 2. The configuration space Ω_Λ associated to a d -dimensional Ising (or spin-glass) model, defined on a finite volume $\Lambda \subseteq \mathbb{Z}^d$ with *free-boundary conditions*, is given by $\Omega_\Lambda := \{-1, 1\}^\Lambda$, such that a configuration $\omega \in \Omega_\Lambda$ is thus of the form $\omega = (\omega_\ell)_{\ell \in \Lambda}$. The *fundamental degree of freedom* associated to the model is the *spin* at a vertex $\ell \in \Lambda$, which is the random variable $\sigma_\ell : \Omega_\Lambda \rightarrow \{-1, 1\}$ defined by $\sigma_\ell(\omega) := \omega_\ell$, for all $\ell \in \Lambda$. The Hamiltonian function associated to each configuration is determined by

$$\mathcal{H}_\Lambda(\omega; \beta, |\mathbf{H}|) := -\beta \sum_{\{i,j\} \in \mathcal{E}(\Lambda)} \sigma_i(\omega) \sigma_j(\omega) - |\mathbf{H}| \sum_{i \in \Lambda} \sigma_i(\omega), \quad (1)$$

where $\beta \geq 0$ is the *Boltzmann inverse absolute temperature*, $|\mathbf{H}|$ the modulus of the magnetic-field, and $\mathcal{E}(\Lambda) := \{\{i, j\} \subset \Lambda : i \sim j\}$ the set of edges associated to the lattice Λ . Finally, the Gibbs distribution of the Ising model in Λ with the free-boundary condition, at parameters β and $|\mathbf{H}|$, is the probability-distribution density on Ω_Λ given by:

$$\rho_\Lambda(\omega; \beta, |\mathbf{H}|) := \frac{1}{\mathcal{Z}_\Lambda(\omega; \beta, |\mathbf{H}|)} \exp(-\mathcal{H}_\Lambda(\omega; \beta, |\mathbf{H}|)), \quad (2)$$

¹Also called the *cost function*.

wherein:

$$\mathcal{Z}_\Lambda(\omega; \beta, |\mathbf{H}|) := \sum_{\omega \in \Omega_\Lambda} \exp(-\beta \mathcal{H}_\Lambda(\omega; \beta, |\mathbf{H}|)), \quad (3)$$

defines the *partition function* of the statistical mechanical system.

However, solving the partition function analytically for most quantum field theories and statistical mechanical systems poses a formidable challenge. Consequently, the adiabatic theorem is introduced. In classical dynamical systems, an adiabatic transformation is a canonical diffeomorphism in phase-space, specifically a diffeomorphism preserving the canonical symplectic form on the cotangent-bundle of the configuration space manifold. This transformation is also a phase-space homeomorphism, ensuring that the topological invariants of the phase-space manifold remain constant after an adiabatic transformation.

Definition 3. *Classical ergodic and Hamiltonian dynamical systems.* For more details, cf. refs. [11, 20, 22, 17].

1. A classical ergodic dynamical system is an ordered list $\langle \Omega, \mathcal{F}, \mu, \Phi \rangle$, such that $\langle \Omega, \mathcal{F}, \mu \rangle$ is a probability space and $\Phi : \Omega \times \mathbb{R} \longrightarrow \Omega$ a flow² on Ω such that $\mu(\Phi_t(A)) = \mu(A)$ for all $A \subseteq \Omega$ and $t \in \mathbb{R}$, and, whenever $E \in \mathcal{F}$ is such that $\mu(\Phi_{-s}(E) \Delta E) = 0$ for each $s \in \mathbb{R}$, then either $\mu(E) = 0$ or $\mu(E) = \mu(\Omega) = 1$.
2. A Hamiltonian dynamical system with n -degrees of freedom is characterised by an ordered triple $\langle \mathcal{M}, \omega, \mathcal{H} \rangle$, where \mathcal{M} is an n -dimensional differentiable manifold representing the *configuration space*, $\omega \in \sec \bigwedge^2 T^* \mathcal{M}$ is the *canonical symplectic 2-form* on the co-tangent bundle of \mathcal{M} (modelling the *phase-space* of the system) and $\mathcal{H} \in \mathcal{C}^1(\mathcal{M}, \mathbb{R})$ is the *Hamiltonian or energy function* generating the dynamics on \mathcal{M} . The natural volume element defined on the phase-space is the Liouville $2n$ -form $\vartheta := (1/n!) \omega^{\wedge n} \in$

²Let \mathcal{M} be a differentiable manifold and $T \subset \mathbb{R}$ an open interval containing $t_0 := 0$. A mapping $\Psi : \mathcal{M} \times T \longrightarrow \mathcal{M}$ is called a flow if and only if $t \in T \mapsto \Psi(x, t)$ is continuous, for each $x \in \mathcal{M}$ fixed, and $y \in \mathcal{M} \mapsto \Psi_s(y) := \Psi(y, s)$ is a diffeomorphism, for each $s \in T$.

$\sec \bigwedge^{2n} T(T^* \mathcal{M})$. The Hamiltonian vector-field $\mathbf{X}_{\mathcal{H}} \in \mathcal{X}(T^* \mathcal{M})$ associated to the energy function \mathcal{H} is the unique vector-field on the phase-space obeying the constraint:

$$i_{\mathbf{X}_{\mathcal{H}}} \omega = d\mathcal{H}. \quad (4)$$

Finally, the phase-space flow $\Psi : T^* \mathcal{M} \times \mathbb{R} \longrightarrow T^* \mathcal{M}$ generated by $\mathbf{X}_{\mathcal{H}}$ is the diffeomorphism determined by the following initial-value problem:

$$\Psi(p, 0) = p, \quad (5)$$

$$\left. \frac{\partial}{\partial s} \Psi(p, s) \right|_{s=0} = \mathbf{X}_{\mathcal{H}}(p), \quad (6)$$

for each $p \in T^* \mathcal{M}$, the well-posedness of which follows from Picard–Lindelöf theorem. Note that Eq. (6) can be rewritten as the Lie derivative of the flow Ψ such that:

$$\mathcal{L}_{\mathbf{X}_{\mathcal{H}}} \omega = 0, \quad (7)$$

from which follows that $\Psi_s (s \in \mathbb{R})$ is a symplectomorphism.

3. Let $\langle \mathcal{M}, \omega, \mathcal{H} \rangle$ be a Hamiltonian dynamical system with n -degrees of freedom. A \mathcal{C}^1 -mapping $\theta : T^* \mathcal{M} \longrightarrow T^* \mathcal{M}$ is an *adiabatic transformation* whenever θ is a symplectomorphism such that $\langle T^* \mathcal{M}, \mathbf{B}(T^* \mathcal{M}), \mu, \theta \rangle$ is ergodic, where $\mathbf{B}(T^* \mathcal{M})$ is the Borel σ -algebra of the differentiable manifold $T^* \mathcal{M}$, and:

$$\mathcal{S} \in \mathbf{B}(\mathcal{M}) \mapsto \mu(\mathcal{S}) := \int_{\mathcal{S}} \vartheta \in [0, \infty], \quad (8)$$

is the Lebesgue measure induced by the Liouville volume-element ϑ .

Example 4. The characterisation of an adiabatic transformation in a classical mechanical system is exemplified by the motion of a simple pendulum in a gravitational field. Let us consider the scenario where the height of the pendulum is continually augmented within a time interval significantly exceeding the period of oscillation of the pendulum. During this process, as the distance between the centre of mass of the pendulum and the centre of gravity of the planet increases, the period ex-

tends accordingly. Remarkably, the shape of the trajectories of the pendulum, with respect to its centre of mass, in the phase-space remains unaltered. In other words, the adiabatic transformation operates homeomorphically, mapping one closed orbit onto another whilst keeping the topological invariants unaltered.

In quantum mechanics, the adiabatic theorem [6, 13] states that if the Hamiltonian operator changes on a timescale orders of magnitude greater than the natural period of motion of the system, and the system is initially prepared in an eigenstate of the Hamiltonian operator, it will persist in that eigenstate after the adiabatic transformation.

In order to elucidate the aforementioned assertions with precision, we shall state and prove an elementary version of the quantum adiabatic theorem in a modern form, as discovered by M. Berry [5, 3, 4] and B. Simon [19]. The seminal paper wherein the theorem was initially discovered, by M. Born and V. Fock, is referenced at [6].

Theorem 5. *Consider the time evolution of a quantum mechanical system, with its state space modelled on a Hilbert space \mathfrak{H} . Let this evolution be governed by a time-dependent Hamiltonian operator $\mathcal{H}(t) : \mathfrak{H} \longrightarrow \mathfrak{H}$ for $t \geq 0$, such that:*

$$\mathcal{H}(t) = \mathcal{H}_0 + \varepsilon g(t) \mathcal{V}, \quad (9)$$

where \mathcal{H}_0 is a Hermitian operator referred to as the free Hamiltonian, \mathcal{V} is a Hermitian operator representing the interaction potential, $\varepsilon > 0$ is the parameter dictating the strength of the coupling between the free Hamiltonian and the potential, and $t \mapsto g(t)$ is a differentiable, real-valued, monotonically increasing function. We designate the scenario in which $\varepsilon \rightarrow 0^+$ as the adiabatic limit of the quantum mechanical system under consideration. Moreover, let us posit that the spectrum of the Hamiltonian operator at the initial time, $\mathcal{H} := \mathcal{H}(t_0)$, is unbounded from above and manifests a discreteness:

$$\{E_1, E_2, \dots\} := \text{Spec}(\mathcal{H}) = \mathbb{C} \setminus \{\lambda \in \mathbb{C} : \exists (\mathcal{H} - \lambda \mathbb{I})^{-1}\}, \quad (10)$$

and that there is a spectral gap Δ such that:

$$0 < \Delta \leq |E_n - E_m|, \quad \forall n \neq m.$$

Thus, considering $t \mapsto |\psi(t)\rangle \in \mathfrak{H}$ as the Schrödinger picture vector representing the quantum state of our system, whenever $|\psi(t_0)\rangle$ is an instantaneous energy eigenstate of $\mathcal{H}(t_0)$ in the adiabatic limit, we assert that $|\psi(t_0)\rangle$ persists in an energy eigenstate of $\mathcal{H}(t)$ for all $t \geq t_0$.

Proof. Without loss of generality, let $t_0 = 0$. Let $|\Phi_n(t)\rangle$ ($n \in \mathbb{N}$) be the family of instantaneous energy-eigenvectors of the time-varying Hamiltonian operator $\mathcal{H}(t)$, corresponding to the eigenvalues $E_n(t)$ ($n \in \mathbb{N}$), such that the following eigenvalue equation is obeyed:

$$\mathcal{H}(t) |\Phi_n(t)\rangle = E_n(t) |\Phi_n(t)\rangle. \quad (11)$$

The Sturm–Liouville theory, and the Hermiticity of $\mathcal{H}(t)$, guarantees the completeness of the orthogonal set $\{|\Phi_n(t)\rangle\}_{n \in \mathbb{N}}$ of energy-eigenvectors spanning the Hilbert space \mathfrak{H} . Let $t \in \mathbb{R} \mapsto |\psi(t)\rangle \in \mathfrak{H}$ be the Schrödinger-picture state-vector describing the evolution of our quantum mechanical system, obeying the Schrödinger equation:

$$i\hbar \partial_t |\psi(t)\rangle = \mathcal{H}(t) |\psi(t)\rangle. \quad (12)$$

The completeness of the set of energy-eigenstates entails that the state vector $|\psi(t)\rangle$ can be expressed as a linear combination of the energy-eigenvectors in the subsequent manner:

$$|\psi(t)\rangle = \sum_{n \in \mathbb{N}} c_n(t) e^{-\frac{i}{\hbar} \int_0^t ds E_n(s)} |\Phi_n(t)\rangle. \quad (13)$$

Now, let us examine the total time-derivative of the eigenvalue equation, denoted as

Eq. (11), yielding:

$$\dot{\mathcal{H}}(t) |\Phi_n(t)\rangle + \mathcal{H}(t) \partial_t |\Phi_n(t)\rangle = \dot{E}_n(t) |\Phi_n(t)\rangle + E_n(t) \partial_t |\Phi_n(t)\rangle. \quad (14)$$

Henceforth, by computing the inner product of the aforementioned equation with the energy-state vector, we ascertain the ensuing identity:

$$[E_m(t) - E_n(t)] \langle \Phi_m(t) | \partial_t |\Phi_n(t)\rangle \quad (15)$$

$$= \dot{E}_n(t) \delta_{mn} - \langle \Phi_m(t) | \dot{\mathcal{H}}(t) | \Phi_n(t) \rangle \quad (16)$$

Therefore, for any pair of indices $(n, m) \in \mathbb{N} \times \mathbb{N}$ such that $n \neq m$, it follows that:

$$\langle \Phi_m(t) | \partial_t |\Phi_n(t)\rangle = -\frac{\langle \Phi_m(t) | \dot{\mathcal{H}}(t) | \Phi_n(t) \rangle}{E_m(t) - E_n(t)}. \quad (17)$$

Upon substituting the linear expansion of the state vector $|\psi(t)\rangle$, as articulated in Eq. (13), into the Schrödinger equation (12), one infers that:

$$\dot{c}_m(t) = -c_m(t) \langle \Phi_m(t) | \partial_t |\Phi_m(t)\rangle \quad (18)$$

$$- \sum_{n \neq m} c_n(t) e^{-\frac{1}{\hbar} \int_0^t ds [E_m(t) - E_n(t)]} \langle \Phi_m(t) | \partial_t |\Phi_n(t)\rangle. \quad (19)$$

Let us now substitute Eq. (17) into Eqs. (18, 19) to yield the ensuing first-order differential equation governing the coefficients $c_n(t)$:

$$\dot{c}_m(t) = -c_m(t) \langle \Phi_m(t) | \partial_t |\Phi_m(t)\rangle \quad (20)$$

$$+ \sum_{n \neq m} \frac{c_n(t) e^{-\frac{1}{\hbar} \int_0^t ds [E_m(t) - E_n(t)]} \langle \Phi_m(t) | \dot{\mathcal{H}}(t) | \Phi_n(t) \rangle}{E_m(t) - E_n(t)}. \quad (21)$$

However, it is imperative to bear in mind that $\dot{\mathcal{H}}(t) = \varepsilon \dot{g}(t) \mathcal{V}$. Consequently, considering the adiabatic limit (wherein $\varepsilon \rightarrow 0$) in Eqs. (20, 21) entails the equation

of motion:

$$c_m(t) = c_m e^{i\gamma_m(t)}, \quad c_m := c_m(0), \quad (22)$$

where:

$$\gamma_m(t) := i \int_0^t ds \langle \Phi_m(s) | \partial_s | \Phi_m(s) \rangle \quad (23)$$

represents the so-called *geometric phase*. (For a historical introduction, we refer to [3, 4]. To delve into contemporary issues within the framework of the Aharonov–Bohm effect, consult [16, 1]). Therefore, bearing in mind the projection of the state–vector $|\psi(t)\rangle$ onto the instantaneous energy–eigenstates, given by Eq. (13), we ultimately deduce that:

$$|\psi(t)\rangle = \sum_{n \in \mathbb{N}} c_n e^{i[\gamma_n(t) - \frac{1}{\hbar} \int_0^t ds E_n(s)]} |\Phi_n(t)\rangle. \quad (24)$$

From Eq. (24), we deduce that if the initial state–vector $|\psi(0)\rangle$ begins in an energy–eigenstate of the Hamiltonian operator $\mathcal{H}(0)$ at $t = 0$, it will persist in an energy–eigenstate of the Hamiltonian operator $\mathcal{H}(t)$ at any subsequent time $t > 0$, as asserted. **QED.**

Remark 6. Let us briefly expound upon the rationale underpinning the nomenclature bestowed upon $\gamma_n(t)$ as the “geometric phase.” Consider the scenario in which the state $|\psi(t, \xi)\rangle$ of our quantum mechanical system is parametrised by a local coordinate system $\xi := (\xi^\mu)$ within a chart belonging to the atlas of a differentiable manifold \mathcal{M} that models the parameter space. Furthermore, let $\mathcal{C} : t \in [0, 1] \mapsto x(t) \in \mathcal{M}$ be a homotopy belonging to the fundamental group based at a point x , such that $\mathcal{C} \in \pi_1(x)$, and assume that the image of \mathcal{C} is encompassed by the domain of the chart ξ . Consequently, employing D/Ds to represent the Fréchet derivative on the sections of the tangent–bundle of \mathcal{M} with respect to the tangent

vector of the curve $t \mapsto x(t)$, we can recast Eq. (23) in the ensuing fashion:

$$\gamma_m(t) := i \int_0^t ds \langle \Phi_m(x(s)) | \frac{D}{Ds} | \Phi_m(x(s)) \rangle \quad (25)$$

$$= i \int_0^t ds \frac{\partial(\xi^\mu \circ x(s))}{\partial s} \langle \Phi_m(x(s)) | \frac{\partial | \Phi_m(x(s)) \rangle}{\partial \xi^\mu} \rangle \quad (26)$$

$$i \int_{\mathcal{C}} d\xi^\mu \langle \Phi_m(\xi) | \frac{\partial | \Phi_m(\xi) \rangle}{\partial \xi^\mu} \rangle. \quad (27)$$

Now, it is worth noting that a Hilbert space-valued connection differential 1-form $\mathcal{A}^{(n)} \in \mathfrak{H} \otimes \sec \bigwedge^1 T\mathcal{M}$, known as the Berry connection, can be constructed. In local coordinates:

$$\mathcal{A}^{(n)} := d\xi^\mu \wedge \left(\langle \Phi_n(\xi) | \frac{\partial | \Phi_n(\xi) \rangle}{\partial \xi^\mu} \right), \quad (28)$$

where the Einstein summation convention is applied. The associated curvature differential 2-form for this connection is thus:

$$\Omega^{(n)} := d\xi^\mu \wedge d\xi^\nu \wedge \left(\frac{\partial \langle \Phi_n(\xi) | \partial | \Phi_n(\xi) \rangle}{\partial \xi^\mu} - \frac{\partial \langle \Phi_n(\xi) | \partial | \Phi_n(\xi) \rangle}{\partial \xi^\nu} \right). \quad (29)$$

Therefore, by virtue of Stokes' theorem, it becomes evident from the aforementioned expressions that the geometric phase is, indeed, the *homotopy* of the Berry connection:

$$\gamma_m[\mathcal{C}] = \int_{\Sigma} \Omega^{(m)}, \quad (30)$$

where $\Sigma \subset \mathcal{M}$ is any differentiable submanifold for which $\partial\Sigma = \mathcal{C}$.

The quantum adiabatic optimisation algorithm [9, 18, 7] involves decomposing the Hamiltonian operator into a “free” term that can be analytically solved, and an “interaction” potential. The interaction potential is activated gradually, allowing the ground-state solution of the complete Hamiltonian to offer a solution to the optimisation problem. The vacuum energy, critical in this process, can be computed using the adiabatic theorem.

Let us make the above assertions precise. For more details on quantum computation and quantum information, cf. Ref. [15] for a comprehensive exposition. An adiabatic quantum algorithm to solve a combinatorial optimisation problem \mathcal{P} (recall Def. (1)) with objective function $f(\omega)$, $\omega \in \Omega$, works on a register Q of n -qubits having superposition state $|\psi_t\rangle$ at a time t . The algorithm is described by a one-parameter family of Hamiltonian operators, $t \mapsto \mathcal{H}(t)$, where the parameter t is identified with time, and specified by the following components:

1. A “free” or initial Hamiltonian \mathcal{H}_0 , chosen such that the ground-state of the system can be solved analytically.
2. An interacting, also called “problem,” Hamiltonian \mathcal{H}_I that encodes the objective function such that the ground state of Q is an eigenstate of \mathcal{H}_I having minimum energy-eigenvalue. In other words, a ground-state of Q corresponds to an optimal solution to \mathcal{P} .
3. An adiabatic evolution path, a function $s : t \mapsto s(t)$ that is monotonically decreasing from 1 to 0 as $t \in [0, T]$, where T is the so-called “total elapsed-time” of the adiabatic evolution.

Thence, the total Hamiltonian operator $\mathcal{H}(t)$ creates a gradual transition from \mathcal{H}_0 to \mathcal{H}_I according to $\mathcal{H}(t) := s(t)\mathcal{H}_0 + (1 - s(t))\mathcal{H}_I$. The Hermitian operator $\mathcal{H}(t)$ is, therefore, referred to as the adiabatic quantum algorithm for solving the combinatorial optimisation problem \mathcal{P} .

For a modern review discussing the field of quantum adiabatic computation, cf. ref. [2].

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