Homological Description of the Quantum Adiabatic Evolution With a View Toward Quantum Computations

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Abstract

We import the tools of Morse theory to study quantum adiabatic evolution, the core mechanism in adiabatic quantum computations (AQC). AQC is computationally equivalent to the (pre-eminent paradigm) of the Gate model but less error-prone, so it is ideally suitable to practically tackle a large number of important applications. AQC remains, however, poorly understood theoretically and its mathematical underpinnings are yet to be satisfactorily identified. Through Morse theory, we bring a novel perspective that we expect will open the door for using such mathematics in the realm of quantum computations, providing a secure foundation for AQC. Here we show that the singular homology of a certain cobordism, which we construct from the given Hamiltonian, defines the adiabatic evolution. Our result is based on E. Witten’s construction for Morse homology that was derived in the very different context of supersymmetric quantum mechanics. We investigate how such topological description, in conjunction with Gauß-Bonnet theorem and curvature based reformulation of Morse lemma, can be an obstruction to any computational advantage in AQC. We also explore Conley theory, for the sake of completeness, in advance of any known practical Hamiltonian of interest.

Key words: Quantum adiabatic evolution, Gradient flows, Morse homology, Gauß-Bonnet theorem, Dupin indicatrix.
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1 Introduction

Quantum algorithms running on quantum computers promise to solve computational problems that are intractable for classical computers. A salient illustration of this computational supremacy is Shor’s algorithm [20], which solves prime factorization in polynomial time whereas the best classical algorithm takes an exponential time. Grover’s algorithm [10], which searches a marked item in large unsorted datasets, is another example that comes with quadratic speed-up over classical counterparts. These two examples were instrumental in the subsequent effervescence around quantum computing.

Today, quantum computing research is dichotomized essentially around two paradigms: the gate model [17] and adiabatic quantum computing (AQC) [9]. While the gate model possesses robust mathematical foundations, AQC lacks such foundations and a deep understanding of its power. This is unfortunate, because AQC is not only computationally equivalent to the gate model [1, 16, 14], but also less error-prone [6, 12] and much easier to use for a large number of important applications (binary optimization problems—an AQC processor is, in fact, an optimizer).

The present paper fills that lacuna – and lays the required foundation – by offering a completely novel mathematical depiction of AQC based on beautiful mathematics: Morse theory. Our topological investigation unveils hidden mathematical structures underlying AQC’s core mechanism: quantum adiabatic evolution. The arsenal of tools that comes with such mathematics—such as gradient flows, Morse homology and Gauß-Bonnet theorem—are weapons we deploy to quantify essential aspects of the adiabatic evolution.

1.1 What is a Morse Function?

A Morse function is a function whose critical points are non degenerate. Consider, for instance, the real-valued function

\[ f(s, \lambda) = \lambda^2 - s^2. \] (1.1)

Its graph is the saddle surface depicted in Figure 1. A critical point of \( f \) is a point \( p = (s, \lambda) \), where the gradient of \( f \) vanishes; that is, a point at which \( \partial_s f(p) = \partial_\lambda f(p) = 0 \), which yields, the point \( p = (0, 0) \) in this example. This critical point is non degenerate because the determinant of the Hessian of \( f \) at \( p \) is not zero. In fact, the Hessian of \( f \) is given by the matrix

\[
\begin{pmatrix}
\partial_{ss} f(s, \lambda) & \partial_{s\lambda} f(s, \lambda) \\
\partial_{s\lambda} f(s, \lambda) & \partial_{\lambda\lambda} f(s, \lambda)
\end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}.
\] (1.2)

It has two non-zero eigenvalues of opposite signs, in which case the critical point \( p \) is called a saddle point. A non degenerate critical point with strictly negative eigenvalues (of the Hessian) is called a maximum (or a source). For instance, \((0, 0)\) is a maximum for the function \( f(s, \lambda) = -\lambda^2 - s^2 \) (the graph of which is the reversed bowl in Figure 3 (c)). Similarly, a non degenerate critical point with strictly positive eigenvalues is called a minimum (or a sink) (e.g., Figure 3 (a)).

1.2 A Primer on Morse Theory

Morse theory stems from the observation that important topological properties of smooth manifolds can be obtained from the critical points of smooth functions on them. To un-
Figure 1: Graph of the function $f(s, \lambda) = \lambda^2 - s^2$.

To understand this, let $M$ be a manifold with—possibly empty—boundaries $M_0$ and $M_1$; a Morse theorist would say $M$ is a cobordism from $M_0$ to $M_1$ and denote it by $(M, \partial M)$, where $\partial M = M_0 \sqcup M_1$. Figure 2 gives two examples of cobordisms with two different topologies. The one on the left (tea pot-like) has an empty boundary (i.e., is a closed surface), and the one on the right has a non empty boundary ($M_0$ is the lower circular boundary and $M_1$ is the disjoint union of the two upper circular boundaries). In Figure 2 (left), the height function is Morse and has four non degenerate critical points: a minimum, a saddle point, and two maxima. On the second surface, Figure 2 (right), the height function is also Morse, only with one critical point: a saddle point.

M. Morse’s key observation is that, with the knowledge of critical points, it is possible to reverse engineer the original topology. The tool for that is the powerful handlebodies decomposition procedure, which we use repeatedly in this paper. Figure 3 provides the dictionary between the critical points and the handles that one can use to recover the cobordism on which the Morse function is defined. For instance, the surface on Figure 1 (left) is recovered by glueing a 0-handle, 1-handle, and two 2-handles, corresponding to the minimum, the saddle point, and the two maxima, respectively.

![Figure 2: (Left) Deformed Sphere. The height function is Morse and has four critical points. (Right) The so-called pair of pants has a different topology (with Euler characteristic $\chi = \#\text{minima} - \#\text{saddles} + \#\text{maxima} = -1$, compared to 2 for the sphere). The height function is also Morse but has only one critical point. The pair of pants is the cobordism that is assigned to Grover’s search Hamiltonian.](image)

In the language of homology, the relation between the topology of $M$ and the critical points
is expressed with the so-called Morse inequalities, where the Betti number $\beta_i$ of the singular homology of $M$ gives an upper bound for the number of critical points of index $i$. (A good reference for the algebraic topological notions employed here – such as homology, Betti numbers, and Euler characteristic – is the excellent book [4] which is also our main reference for Morse theory). In the example of the closed surface of Figure 1, one has $\beta_1 = 0$ (since the surface is a continuous deformation of the 2 dimensional sphere and thus contains no hole), which indicates that the saddle point can be canceled with a better choice of Morse function (e.g., by projecting onto the horizontal axis). The pair of pants, however, has $\beta_1 = 2$, indicating that the saddle point there can not be canceled by any continuous deformation.

The full power of Morse theory was unleashed by R. Thom and S. Smale (the latter with his work on the Poincaré conjecture) in the sixties and subsequently, in the eighties, by E. Witten. S. Smale introduced the dynamical system point of view which has played a central role since then; in particular, in Witten’s explicit construction of the Morse complex [24]. To the Morse function $f$ we assign the (downward) gradient flow given by

$$x'(\tau) = - (\nabla f) \circ x(\tau) \quad (1.3)$$

for smooth curves $x(\tau) \in (M, \partial M)$. The trajectories (called instantons in [24]) define a complex whose homology turns out to be isomorphic to the singular homology of the given manifold. This is the apex result of Morse theory, known as the Morse homology theorem, which plays a central role in this paper. Another major development, due C. Conley, is the generalization to degenerate critical points [7]. His observation is that many of the constructions can be carried out with a less local approach. In particular, the behaviour of trajectories around a critical point is indicative of its nature. Therefore, it suffices to consider isolated neighbourhoods around critical points. Within such neighbourhood, continuous deformations can split the degenerate critical into a set of non degenerate points without changing the dynamics around the isolated neighbourhood. The interest is then on how trajectories connect the isolated neighbourhoods of the function $f$. We briefly explore this towards the end of the paper.

1.3 Goal of The Paper and Summary of The Results

In the present paper we import the tools of Morse theory to study quantum adiabatic evolution, where we describe topologically, the adiabatic solutions of the Schrödinger equation ($\hbar$ is set to 1):

$$i \frac{\partial}{\partial t} |\varphi(t)\rangle = H(t)|\varphi(t)\rangle. \quad (1.4)$$
Adiabatic solutions, central to AQC, are solutions obtained after passing to the slow regime $(s = \varepsilon t$ with $0 < \varepsilon < 1$) at the singular limit $\varepsilon \rightarrow 0$. Here $H(t)$ is some Hamiltonian of interest operating on the Hilbert space $\mathcal{H} = \mathbb{C}^{2^n}$. We assume usual smoothness assumptions on $H(t)$ and $H'(t)$ and their spectral projections.

Our topological expedition starts with the consideration of the function

$$f(s, \lambda) = \det(H(s) - \lambda I),$$

that is, the characteristic polynomial of the Hamiltonian $H(s)$ in the slow regime. Our results are ramifications of this choice of the function $f$. In particular, if $f$ is Morse, then Morse theory is applied without difficulty, resulting in a number of direct topological reformulations of the quantum mechanical objects. Indeed, we automatically inherit a gradient flow given by the Morse function $f$. This gradient flow is defined on a cobordism $(M, \partial M)$ that is also straightforwardly inherited from the critical points of $f$ using the handlebodies decomposition. The eigenenergies (energies of the adiabatic solutions), which are defined by $f(s, \lambda) = 0$, manifest themselves as level sets of the gradient flow. As a matter of fact, in the light of the Morse homology theorem, these level sets are subjected to the singular homology of the cobordism $(M, \partial M)$. These connections are the flow trajectories, and by orthogonality, we obtain the level sets, in particular, the eigenenergies. We extend these results to degenerate critical points in the case of the so-called $k-$fold saddle points. Conley theory can be applied, as well, without major difficulties, leading to same conclusions as in the non degenerate case.

Our voyage doesn’t end here. We start our descent from the topological global description to a local description of the quantum adiabatic evolution around the critical points of $f$. Essential to our local description is the curvature at the critical points: two Hamiltonians having the same topology are not necessarily “computationally equivalent” i.e., have different speedups. We use differential geometry to obtain the quantitative behaviour of the eigenenergies around the critical points. In fact, given the homology of the cobordism $(M, \partial M)$, Gauß-Bonnet theorem distributes the Gaussian curvature of $(M, \partial M)$ consistently with this homology—but not necessarily in the same way for topologically equivalent Hamiltonians. By re-expressing Morse lemma in terms of the principal curvatures, one can obtain the delay factor at the given critical point. We explain the role of the shape operator to describe the adiabatic evolution—including the quantitative behaviour of the eigenenergies. In fact, since the shape operator is Hermitian (self-adjoint), one might think of this procedure as dimensionality reduction of the original Hamiltonian $H(s)$.

1.4 An Illustrative Example: Quantum Search

As an introductory example, let us consider the adiabatic Hamiltonian for the search problem [18, 22]:

$$H(s) = (1 - s)H_{\text{initial}} + sH_{\text{final}},$$

where $s = t/T$, with $T > 0$, and

$$H_{\text{initial}} = 1 - |\hat{0}\rangle\langle\hat{0}|,$$

$$H_{\text{final}} = \sum_{z \in \{0,1\}^n - \{u\}} |z\rangle\langle z| = 1 - |u\rangle\langle u|.$$
As usual, the notations $\{|z\rangle\}_{z \in \{0,1\}^n}$ and $\{|\tilde{z}\rangle\}_{z \in \{0,1\}^n}$ stand for the computational and Hadamard bases, respectively. The state $|u\rangle$ is the sought item (the unsorted database being the computational basis $\{|z\rangle\}_{z \in \{0,1\}^n}$). The search problem can be put into the two-dimensional subspace spanned by the two states $|v\rangle := |\tilde{0}\rangle - 1/\sqrt{N}|u\rangle$ and $|u\rangle$, with $N = 2^n$. In this orthogonal basis, the restricted Hamiltonian $H(s)$ takes the form

$$H(s) = \begin{pmatrix} \frac{(1-s)(N-1)}{N} & \frac{-(1+s)(N-1)}{N^{3/2}} \\ \frac{s-1}{\sqrt{N}} & \frac{1-s+sN}{N} \end{pmatrix}.$$  \hspace{1cm} (1.9)

The characteristic polynomial of this $2 \times 2$ matrix is

$$f(s, \lambda) = \frac{(N-1)}{N} (s-s^2) + \lambda^2 - \lambda,$$  \hspace{1cm} (1.10)

and has one critical point $p$ obtained by equating its partial derivatives to zero. This critical point is non degenerate because the eigenvalues $k_1(p) := -2 (N-1)/N$ and $k_2(p) := 2$ of the Hessian of $f$ are non zero, and because $k_1(p)k_2(p) < 0$, the critical point is a saddle point. Now, the graph of the function $f$ (see Figure 1) comes with a Gaussian curvature $K(s, \lambda) = (f_{ss}f_{\lambda\lambda} - f_s^2)/((1 + f_s^2 + f_{\lambda}^2)^2)$. Gauß-Bonnet theorem forces this curvature to distribute itself on the surface consistently with this topology (consistent with Euler characteristic -1). In fact, the curvature is “dumped” at the critical point $p$:

$$\int_{(M,\partial M)} K(s, \lambda) d\sigma \sim \int_{V(p)} K d\sigma = -2\pi + O(1/N),$$  \hspace{1cm} (1.11)

where $V(p)$ is an arbitrary small neighbourhood around the saddle point $p$, and independent of $n$.Explicitly, we have, $K(p) = k_1(p)k_2(p) = -4(1 - \frac{1}{N})$ and the two quantities $k_1(p)$ and $k_2(p)$ are the two principal curvatures of the saddle surface at $p$. If we intersect the surface with planes horizontal to the tangent plane $T_pM$, in particular the plane $f(s, \lambda) = 0$, we obtain two hyperbola called Dupin indicatrix. The radius $g(s)$ of this indicatrix (that is, the distance between the two hyperbola), which is also the energy difference, is constrained by the amount of curvature at $p$. Indeed, we have

$$g(s) = 2 \frac{-k_2(p)}{k_2(p)} \frac{\left(2f(p) + k_1(p)(s - \frac{1}{2})^2\right)}{k_2(p)},$$  \hspace{1cm} (1.12)

and from which we infer:

$$\int_0^1 \frac{ds}{g(s)^2} = \frac{-k_2(p)}{\sqrt{k_1(p)f(p)}} \arctan \left(\frac{\sqrt{k_1(p)}}{\sqrt{8f(p)}}\right) = \frac{\pi}{2} \sqrt{\frac{1}{N}} - 1 + O\left(\frac{1}{\sqrt{N}}\right),$$  \hspace{1cm} (1.13)

which is the total time needed to tunnel through the saddle point $p$ without destroying the adiabaticity. Our approach thus provides a new derivation for quadratic speedup.

### 1.5 Outline of The Paper

The paper is organized as follows. Section 2 reviews the adiabatic theorem. The version we review is valid not only for both discrete and continuous spectrum, but also in the presence of the eigenvalues crossing. In section 3, we summarize properties of gradient flows and review Morse lemma. Section 4 connects the quantum adiabatic evolution to gradient flows. Section
5 has two parts: (1) global description of the quantum adiabatic evolution based on Morse homology, and (2) local description of the Gaussian curvature around the critical points. Gauß-Bonnet theorem bridges the two parts. The last section (Section 6) generalizes the findings of Section 5 to the degenerate case – specifically, to the $k$-fold saddle points. We conclude in Section 7 with some open questions.

| Quantum adiabatic evolution | Morse theory |
|----------------------------|-------------|
| Hamiltonian $H(s)$         | Morse function $f(s, \lambda) = \det(H(s) - \lambda I)$ |
| Eigenenergies              | Level sets of the gradient flow: $x'(\tau) = -(\nabla f) \circ x(\tau)$ |
| Eigenenergies              | are orthogonal to the boundary maps of the Morse homology |
| Spectral gap               | Radius of Dupin Indicatrix |
| Dimensionality reduction of $H(s)$ | The shape operator |
| Degeneracy                 | $k$–fold saddle points |

Table 1: Correspondence between the quantum adiabatic evolution and Morse theory.

2 The Adiabatic Theorem

The adiabatic theorem is an existence result of solutions of the Schrödinger equation that goes back to the early days of quantum mechanics. It describes both the solutions and the regime (i.e., conditions) in which such solutions exist. Physically, this regime is characterized by “slowly” varying the time dependent Hamiltonian. Mathematically, this is done by considering the Schrödinger equation

$$i \frac{\partial}{\partial t} |\varphi(t)\rangle = H(t)|\varphi(t)\rangle,$$  \hspace{1cm} (2.1)

with the new (slow) time $s = \varepsilon t$ with $0 < \varepsilon < 1$ which yields:

$$i \varepsilon \frac{\partial}{\partial s} |\varphi_\varepsilon(s)\rangle = H(s)|\varphi_\varepsilon(s)\rangle.$$  \hspace{1cm} (2.2)

The adiabatic theorem describes solutions at the singular limit $\varepsilon \to 0$. In the literature, there is no single adiabatic theorem, and different theorems focus on different assumptions on the Hamiltonian (5, 13, 11, 3 to cite a few). They do, however, share the following structure 8:
Theorem 1 Let $P(s)$ be a spectral projection of $H(s)$. In the singular limit $\varepsilon \to 0$, the solution $|\varphi_\varepsilon(s)\rangle$ of equation (2.2) with the initial condition $|\varphi_\varepsilon(0)\rangle \in \text{Range} (P(0))$ is subject to
\[
\text{dist} \left( |\varphi_\varepsilon(s)\rangle, \text{Range} (P(s)) \right) \leq O(\varepsilon^\gamma)
\]
(2.3)
for an appropriate value of $\gamma \geq 0$ depending on the assumptions made about $H(s)$.

This formulation is particularly interesting not only because it is valid for discrete and continuous spectrum, but also because it continues to hold in the event of an eigenvalues crossing. Recall that eigenvalues crossing refer to when $H$ has two eigenvalues $\lambda^i$ and $\lambda^j$ that are isolated from the rest of the spectrum and equal to each other at some time $s$. The order of such a crossing is by definition the order of the zero of $\lambda^j(s) - \lambda^i(s)$.

In their original statement of the adiabatic theorem, Fock and Born [5] restricted themselves to Hamiltonians with simple discrete spectrum. They have showed that if the eigenvalues crossing doesn’t happen, then $\gamma \geq 1$; that is, the gap is a smooth function of $\varepsilon$. To see this, suppose the spectral projection $P(s)$ is given by $|\varphi^i(s)\rangle\langle\varphi^i(s)|$ and consider the ansatz
\[
|\varphi_\varepsilon(s)\rangle = \exp \left\{ \phi(s, \varepsilon) \right\} |\varphi^i(s)\rangle
\]
(4.4)
with the complex-valued function $\phi$ required to satisfy $\phi(0, \varepsilon) = 0$. The substitution in the equation (2.2) yields
\[
\varepsilon\partial_s|\varphi^i(s)\rangle + i\varphi^i(s)|\phi(s, \varepsilon)|\varphi^i(s)\rangle = \lambda^i(s)|\varphi^i(s)\rangle.
\]
Assuming $\varepsilon$ is close to 0, the first term of the left hand side can be neglected. Integrating gives
\[
\phi(s, \varepsilon) = -\frac{i}{\varepsilon} \int_0^s \lambda^i(s)ds + O(\varepsilon).
\]
Thus,
\[
|\varphi_\varepsilon(s)\rangle = \exp \left\{ -\frac{i}{\varepsilon} \int_0^s \lambda^i(s)ds \right\} |\varphi^i(s)\rangle + O(\varepsilon).
\]
(2.5)
To see where the crossing comes in, we need to expand this approximation to the first order. Plugging
\[
|\varphi_\varepsilon(s)\rangle = \exp \left\{ -\frac{i}{\varepsilon} \int_0^s \lambda^i(s)ds \right\} (|\varphi^i(s)\rangle + \varepsilon|\zeta(s)\rangle + O(\varepsilon^2))
\]
(2.6)
in the Schrödinger and solving for the function $|\zeta(s)\rangle$ yields
\[
|\zeta(s)\rangle = \sum_{j \neq i} \left( \frac{A(0)}{(\lambda^j(0) - \lambda^i(0))^2} - \exp \left\{ \frac{i}{\varepsilon} (\lambda^j(s) - \lambda^i(s)) \right\} \frac{A(s)}{(\lambda^j(s) - \lambda^i(s))^2} \right) |\varphi^j(s)\rangle
\]
(2.7)
with $A(s) = i \langle \varphi^i(s) | \frac{d}{ds} H(s) | \varphi^j(s) \rangle$. The term of interest is the denominator $(\lambda^j(s) - \lambda^i(s))^2$, which is not defined when eigenvalues crossing occurs – which is also true for the higher terms in $O(\varepsilon^2)$. If the eigenvalues crossing is excluded, the expression (2.6), with $|\zeta(s)\rangle$ given by (2.7), is a well defined solution.
2.1 Eigenvalues Crossings and AQC

As a matter of fact, in their original paper, Born and Fock also studied eigenvalues crossings and obtained expansions similar to (2.5), with $O(\varepsilon)$ replaced with $O(\varepsilon^{1/(m+1)})$, with $m$ the order of the crossing.

$$|\varphi_\varepsilon(s)\rangle = \exp\left\{-\frac{i}{\varepsilon}\int_0^s \lambda^i(s)ds\right\}|\varphi^i(s)\rangle + O(\varepsilon^{1/(m+1)}).$$

(2.8)

The source of this fractional power is that near the crossing point $|\lambda^j(s) - \lambda^i(s)| = s^m$ (See also [11]). That being said, in the context of AQC, where the time dependent Hamiltonian $H(s)$ has a particular form (as in (2.9)), the eigenvalues crossing doesn’t occur if the time $s$ is the only parameter that drives the evolution. This is a corollary of the so-called non-crossing rule (or avoided crossing rule) which is another important early result, due to von Neumann and Wigner [23]. The proof can be found in [21] or in the original paper [23].

**Theorem 2 (Non-crossing rule)** Suppose the Hamiltonian $H$ depends on a number of independent real parameters, and suppose that $H$ has $r$ eigenvalues with multiplicity $m_i$ for $i = 1, \cdots, r$. Assume that no observable commutes with the Hamiltonian. In this case, the number of the free real parameters to fix $H$ is $2^{2n} + r - \sum_{i=1}^r m_i^2$.

Suppose the Hamiltonian is given by

$$H(s) = \alpha(s)H_{\text{initial}} + \beta(s)H_{\text{final}}$$

(2.9)

where $H_{\text{initial}}$ and $H_{\text{final}}$ are non commuting observables, and $\alpha(s)$ and $\beta(s)$ are two functions that control the evolution (e.g., $\alpha(s) = 1 - s$ and $\beta(s) = s$). Suppose $s_0 < s_1$ are two different times such that for all $s \in [s_0, s_1]$ both functions $\alpha(s)$ and $\beta(s)$ are not zero. The theorem above excludes the scenario where $H(s_0)$ has a simple spectrum whilst $H(s_1)$ has a doubly degenerated eigenenergy. To see this, it suffices to count the number of the free real parameters in each case (that is, for $H(s_0)$ and $H(s_1)$) to see that three parameters in $H(s)$ are to be fixed to obtain $H(s_1)$ (fixing $s$ to $s_1$ in addition to two more parameters). Since $\alpha(s)$ and $\beta(s)$ depend only on $s$, such a scenario can not happen. However, when more parameters (at least two more) are involved, the eigenvalues crossing is plausible.

3 Morse Lemma and Gradient Flows

Let $M$ be a cobordism between $M_0$ to $M_1$ and $f : (M, \partial M) \to [0, 1]$ a smooth function.

**Definition 1** Let $p \in M$ be a non degenerate critical point of $f$. The number $\gamma(p)$ of negative eigenvalues of the Hessian of $f$ at $p$ is called the Morse index of $f$ at $p$.

The Morse index is an intrinsic invariant for the homeomorphism group of $M$ (i.e., one-to-one mappings on $M$ continuous in both directions).

**Example 1** In the 2-dimensional case where the Hessian is a 2 by 2 matrix, the index is necessarily in $\{0, 1, 2\}$.

Around its non degenerate critical points, the function $f$ takes a very simple form:
Lemma 1 (Morse lemma) Let \( p \) be a non degenerate critical point of a smooth function \( f : M \to [0,1] \). There exists a neighbourhood \( U \) of \( p \) and a diffeomorphism \( h : (U,p) \to (\mathbb{R}^m,0) \) such that
\[
f \circ h(x_1, \cdots, x_m) = f(c) - \sum_{1 \leq i \leq \gamma(p)} x_i^2 + \sum_{\gamma(p)+1 \leq i \leq m} x_i^2,
\]
with \( m = \dim(M) \).

An immediate corollary of Morse lemma is that the non degenerate critical points of a Morse function are isolated. Another direct consequence is that, in the 2-dimensional case, a critical point with index values 0, 1 and 2, respectively, corresponds to a local minimum, a saddle point, and a local maximum.

Definition 2 The neighbourhood \( U \) and its image \( h(U) \) in Morse lemma are called, respectively, the manifold chart and Morse chart.

Example 2 (Quantum search) Continuing (from the Introduction) with Grover’s search Hamiltonian with \( f(s,\lambda) = (2^{-n} - 1)s^2 + \lambda^2 \), where we have translated the saddle point to the origin. Figure 4 (a) gives the Morse chart around the origin. Figure 4 (b) gives the manifold chart.

Let \( X \) be a smooth vector field on the cobordism \( M \); that is,
\[
X = \sum_{i=1}^{m} \xi_i(x) \partial_{x_i} \tag{3.1}
\]
where \( x = (x_1, \cdots, x_m) \) coordinates \( M \) and \( \xi_i \) are smooth functions on \( M \). For \( x^0 \in M \), consider the initial value problem (IVP) for smooth curves \( x : \mathbb{R} \to M \) given by
\[
\frac{dx(\tau)}{d\tau} = X(x(\tau)), \quad x(0) = x^0. \tag{3.2}
\]
Solutions $x(\tau)$ are called trajectories (also flow lines or instantons); their properties are summarized in the following proposition (4):

**Proposition 1** The following assertions are true:

1. the set of all trajectories of the IVP problem (3.2) covers $M$;
2. if $M$ is closed, then the trajectory $x(\tau)$ is defined for all $\tau \in \mathbb{R}$;
3. the limits $\lim_{\tau \to -\infty} x(\tau)$ and $\lim_{\tau \to +\infty} x(\tau)$ are two critical points of $f$ (this gives a procedure to locate critical points: starting anywhere on the manifold $M$ and following the flow);
4. trajectories can escape to the boundary;
5. trajectories intersect only at critical points.

The flow generated by $X$ is the smooth map $\Phi_\tau : \mathbb{R} \times M \to M$, which sends the pair $(\tau, x^0)$ to the point $\Phi_\tau(x^0) = x(\tau)$, where $x(\tau)$ is the solution of the initial value problem (3.2). The set $\{\Phi_\tau\}_{\tau}$ is a one parameter group of diffeomorphisms on $M$ with $\Phi_\tau \Phi_{\tau'} = \Phi_{\tau + \tau'}$. The orbit $O(x^0)$ through $x^0$ is defined by the set $\{\Phi_\tau(x^0) | \tau \in \mathbb{R}\}$.

**Definition 3** The flow associated with $X = -\nabla f = -\sum f_{x_i}(x)\partial_{x_i}$ is called the gradient flow.

For gradient flows, we have two more properties in addition to the ones listed in the above proposition. First, if $x(\tau)$ is a trajectory, then $\frac{d}{d\tau} f(x(\tau)) = -|\nabla f(x(\tau))|^2$, which shows that $f$ is decreasing along trajectories (and zero only at the critical points). Second, at any regular point of the gradient $\nabla f$, trajectories are orthogonal to the level sets $f(x) = \text{constant}$. This second property is manifestly important in the next section.

## 4 Gradient Flows for Quantum Adiabatic Evolution

Let $\{\varphi_\epsilon(s)\}$ be the collection of the adiabatic solutions one gets for the different initial conditions (these solutions are given by (2.5) or (2.8), depending whether eigenvalues crossings occur or not). Our aim now is to assign a gradient flow to this collection of solutions. In fact, the gradient flow we construct below is “orthogonal” to this adiabatic flow, in the sense that the adiabatic solutions are level sets of this gradient flow. As mentioned before, we consider the smooth function $f(s, \lambda) = \text{det}(H(s) - \lambda I)$, which itself gives rise to the gradient flow

$$
\begin{align*}
\frac{d}{d\tau} \lambda(\tau) &= -\partial_\lambda f(\lambda(\tau), s(\tau)), \\
\frac{d}{d\tau} s(\tau) &= -\partial_s f(\lambda(\tau), s(\tau)).
\end{align*}
$$

The function $f$ is defined on a open set $U \subset \mathbb{R}^2$, which we assume big enough to include all the critical point of $f$ (which itself is assumed to not possess critical points at the infinities). Later on, the subset $U$ will be replaced with a cobordism in $\mathbb{R}^3$ constructed from the critical points of $f$, using the handle decomposition procedure. In this case, $U$ will be play the role of a Morse chart. In addition to this picture, we have a similar picture for a Morse chart $V := (U \cap s - \text{axis}) \times \text{span}_\mathbb{R}(\{\varphi_\epsilon\}) \subset \mathbb{R} \times \mathcal{H}$ corresponding to the level sets given by the curves $\{\varphi_\epsilon(s)\}$. Indeed, we can “lift” the function $f$ to $V$ as follows:
with \( h \) being the linear map:

\[
h(s, \varphi) = (s, \langle \varphi(s) | H(s) | \varphi(s) \rangle).
\] (4.2)

In particular, \( g(s, |\varphi_\varepsilon\rangle) = 0 + O(\varepsilon^2) \) for the adiabatic solution \( |\varphi_\varepsilon(s)\rangle \); this is because \( \langle \varphi_\varepsilon(s) | H(s) | \varphi_\varepsilon(s) \rangle = \lambda(s) + O(\varepsilon^2) \). This means that the function \( \hat{f} \) is constant on the adiabatic solutions; that is, the latter are level sets for the gradient flow

\[
\begin{align*}
\frac{d}{d\tau} \varphi^{(j)}(\tau) &= -\partial_{\varphi^{(j)}} g(\varphi(\tau), s(\tau)) \\
\frac{d}{d\tau} s(\tau) &= -\partial_s g(\varphi(\tau), s(\tau)).
\end{align*}
\] (4.3)

Here, \( \varphi^{(j)} \) the \( j \)-th component of the vector \( |\varphi\rangle \in \text{span}_R \{ |\varphi_\varepsilon\rangle \} \).

**Proposition 2** The two flows (4.1) and (4.3) are topologically equivalent.

Recall that two autonomous systems of ordinary differential equations \( x' = f(x), x \in M \) and \( y' = g(y), y \in M' \) are said to be topologically equivalent \([2]\) if there exists a homeomorphism \( h : M \to M', y = h(x) \), which maps solutions of the first system to the second, preserving the direction of time.

**Proof 1** Since the direction of time is preserved (i.e., same independent variable \( \tau \) in both systems) we need only to prove that \( h \) given by (4.2) is a homeomorphism. For that we prove the two systems have the same critical points, which implies that \( h \) is invertible outside this set of critical points. The fact that \( \nabla g(x) = \nabla f(h(x)) \nabla h(x) \) for \( x \in V \) implies that the set of critical points of the dynamical system (4.3) is the union of the set of critical points of (4.1) and the set of critical points of \( h \). By the implicit function theorem, critical points of \( h \) are where \( h \) fails to be injective, i.e., points \( (s, \varphi_i(s)) \) and \( (s, \varphi_j(s)) \) with \( \lambda_i(s) = \lambda_j(s) \). But these correspond to critical points (intersections of level sets) of (4.1). Thus, the two dynamical systems (4.1) and (4.3) have the same critical points.

In this section we assigned two topologically equivalent gradient flows (4.1 and 4.3) to the adiabatic solutions of the Schrödinger equation (2.2). The adiabatic solutions (respectively, their energies) are level curves orthogonal to the integral curves of the gradient flow (4.1) (respectively, 4.3). In the next section, we concentrate on the implication of this perspective when \( f \) is Morse.

5 The Non-Degenerate Case: Morse Theory

The goal of this section is to prove Theorem 3 below, which relates the adiabatic flow associated to the Hamiltonian \( H(s) \) to the topology of a certain cobordism \((M, \partial M)\). Our proof is a direct corollary of the different constructions we have built and shall build below. We start this section with the construction of the cobordism \((M, \partial M)\).
5.1 Handlebodies Decomposition: The Cobordism of The Quantum Adiabatic Evolution

Consider the gradient flow (4.1) where the Morse function \( f(s, \lambda) = \det(H(s) - \lambda I) \) is defined on a open compact set \( U \subset \mathbb{R}^2 \) (the Morse chart), which we have assumed to be big enough to include all the critical points of \( f \) (which themselves are assumed to be non degenerate). We would like to extend the domain of \( f \) to a cobordism \((M, \partial M)\) using the technique of handlebodies decomposition which we review now. Define the sublevel set (also half-space) \( M_c \) to be the set of points of \( M \) at which \( f \) takes values less than or equal to \( c \):
\[
M_c := \{ x \in M \mid f(x) < c \}
\]
Let \( p \) be a non degenerate critical point of \( f \) with index \( \gamma(p) \), and let \( D^i \) denotes the \( i \)-dimensional unit disc \( \{ x \in \mathbb{R}^i \text{such that } |x| \leq 1 \} \). The \( \gamma(p) \)-handle is defined to be the set
\[
D^{\gamma(p)} \times D^{m-\gamma(p)}.
\]
(5.1)

Examples of handles are given in Figure 3. We have the following result (for proof see for instance [15, 4]):

**Proposition 3** Assuming, for sufficiently small \( \varepsilon > 0 \), the only critical value in \([c - \varepsilon, c + \varepsilon]\) is \( c = f(p) \), then the sublevel set \( M_{c+\varepsilon} \) can be obtained from the sublevel set \( M_{c-\varepsilon} \) by attaching the \( \gamma(p) \)-handle.

Now, let us assume that the critical values are such that \( f(p_1) < f(p_2) < \cdots < f(p_k) \). If this is not the case, we may perturb \( f \) in such a way that \( f(p_i) \neq f(p_j) \) if \( i \neq j \) (See for instance Theorem 2.34, Chapter 2 in [15]). Proposition 3 says that starting from the lowest critical value \( f(p_1) \) one can then reverse engineer the manifold by inductively attaching \( \gamma(p_i) \)-handle to the sublevel set \( M_{f(p_{i-1})} \).

Returning to our context of adiabatic evolution we obtain the following proposition:

**Proposition 4** Let \( f(s, \lambda) = \det(H(s) - \lambda I) \). If \( f \) is Morse, then the spectrum of \( H(s) \) corresponds to level sets of the gradient flow (4.1) defined on a cobordism \((M, \partial M)\), which obtained, from the critical points of \( f \), using the handlebodies decomposition procedure.

In the next subsection, will explain how the gradient flow of \( f \) triangulates the cobordism \((M, \partial M)\).

5.2 Morse Homology for Non-Degenerate Quantum Adiabatic Evolution

5.2.1 Transversality and Morse-Smale functions

For completeness, we start by reviewing the notion of Morse-Smale functions. The motivation for this “technical” notion is that not all Morse functions give triangulation of the cobordism \((M, \partial M)\). Such functions need to satisfy an additional requirement: Morse-Smale transversality, which, in reality, is not a major constraint; in general, it suffices to “tilt” the Morse function slightly to obtain Morse-Smale transversality – The height function of a vertical torus is a typical example. In general, a Smale-Morse function is a Morse function \( f : M \to [0, 1] \), where the unstable manifold \( W^u(q) := \{ q \} \cup \{ x \in M \mid \lim_{\tau \to -\infty} \Phi_{\tau}(x) = q \} \) and the stable manifold \( W^s(p) := \{ p \} \cup \{ x \in M \mid \lim_{\tau \to +\infty} \Phi_{\tau}(x) = p \} \) of \( f \) intersect transversally for all \( p \) and \( q \) in \text{critical}(f).
5.2.2 The integers \( n(p, q) \): Counting flow lines

Consider two critical points \( p \) and \( q \) of index \( \gamma(p) = k - 1 \) and \( \gamma(q) = k \) respectively, and assume that the intersection \( W(q, p) = W^u(q) \cap W^s(p) \) is not empty. Let \( x(\tau) : \mathbb{R} \to M \) be a gradient flow line from \( q \) to \( p \):

\[
\frac{d}{d\tau} x(\tau) = -\nabla f(x(\tau)), \quad \lim_{\tau \to -\infty} x(\tau) = q, \quad \lim_{\tau \to \infty} x(\tau) = p.
\]

Now since \( \gamma(q) - \gamma(p) = 1 \), the set (moduli space) \( M(q, p) := W(q, p)/\mathbb{R} \) of flow lines connecting \( q \) and \( p \) is zero dimensional. In fact, it consists of a finite number of elements (Corollary 6.29 [4]). The integer \( n(q, p) \in \mathbb{Z}_2 \) is defined to be the sum mod 2 of these numbers.

5.2.3 Morse chain and homology

Let \( C_k(f) \) be the free abelian group generated by the critical points of index \( k \), and define \( C_* = \bigoplus_k C_k(f) \). The homomorphism \( \partial_k : C_k(f) \to C_{k-1}(f) \) defined by

\[
\partial_k(q) = \sum_{p \in \text{critical}_k(f)} n(q, p)p
\]

is called the Morse boundary operator, and the pair \((C_*, \partial_*)\) is called the Morse chain complex of \( f \). The deep connection between Morse theory and topology is expressed in the following landmark result.

**Proposition 5 (Morse homology theorem)** The pair \((C_*, \partial_*)\) is a chain complex, and its homology is isomorphic to the singular relative homology \( H_*(M, \partial M) \).

**Proof 2** See for instance [4] Theorem 7.4.

**Example 3 (Deformed sphere – Figure 5)** We have the chain complex

\[
0 \to \text{span}_{\mathbb{Z}_2}(p_3, p_4) \to \text{span}_{\mathbb{Z}_2}(p_2) \to \text{span}_{\mathbb{Z}_2}(p_1) \to 0,
\]

with the boundary maps \( \partial_4 = \partial_3 = p_2 \) and \( \partial_2 = 2p_1 \mod 2 = 0 \). There are flow lines connecting the two maxima to the minimum (not drawn below) but these ones are not part of the definition. We obtain \( \beta_0 = 1, \beta_1 = 0, \) and \( \beta_2 = 1 \).

Let us remark that, although, we have used \( \mathbb{Z}_2 \) as the field of coefficients, Morse homology theorem holds with coefficients in any commutative ring with unity \( K \). The theorem is proved for \( \mathbb{Z} \), the ring of integers and by a universality argument the proof extends to any commutative ring with unity. When counting the numbers \( n(p, q) \in \mathbb{Z} \), a notion of orientation is introduced. Now, our main result of this section is the following:

**Theorem 3** Let \( f(s, \lambda) = \det(H(s) - \lambda I) \), assumed to be Morse, and let \((M, \partial M)\) be the associated cobordism constructed in Proposition 4. The adiabatic flow associated with \( H(s) \) is uniquely defined by the set critical \( (f) \) and the singular homology \( H_*(M, \partial M; K) \).

**Proof 3** The boundary maps \( \partial_k \) of the Morse complex are uniquely defined by the isomorphism in the Morse homology theorem, in addition to the set of critical points of \( f \). Additionally, Morse lemma gives \( f \) and the gradient flow lines, locally around each critical point. The number \( n(p, q) \) allows us to connect these trajectories consistently. The adiabatic solutions are then level sets of this gradient flow.
In the remainder of this section, we start our descent from the global qualitative description of the quantum adiabatic evolution, given by the theorem above, to a local quantitative description around the critical points of $f$. Essential in our local description is the curvature at the critical points. The reason for moving to this curvature based local description is the fact that two Hamiltonians giving the same topology are not necessarily “computationally equivalent” i.e., have the same speedup. Indeed, Gauß-Bonnet theorem may distribute the total curvature that comes with this topology differently around the critical points, thus, potentially yielding different “speeds”.

### 5.3 Differential Geometry

We first, review some important constructs in differential geometry of surfaces [8].

#### 5.3.1 Gauß map and its derivatives

Let $S$ be a surface in the Euclidean space $\mathbb{R}^3$ and $p$ a point in $S$. We write $n : S \rightarrow \mathbb{S}^1$ for the Gauß map which sends $p$ to the normal (unit) vector $n(p)$. The rate of change of $n$ on a neighbourhood of $p$ measures how rapidly the surface $S$ is pulling away from the tangent plane $T_p S$. Formally, this rate of change is given by the shape operator

$$d(n)(p) : T_p S \rightarrow T_{n(p)} \mathbb{S}^1,$$

which is a Hermitian operator. The determinant of $d(n)(p)$, denoted $K(p)$, is the Gauß curvature at $p$, and its eigenvalues, denoted by $k_1(p)$ and $k_2(p)$, are the two principal curvatures at $p$. (These are generalizations, to surfaces, of the notion of the curvature of a curve. In particular, the principal curvatures are the minimum and the maximum of all curvatures of
all curves on the surface passing through \( p \). The corresponding eigenvectors, called principal directions, \( e_1 \) and \( e_2 \). They form a convenient orthonormal basis for the tangent plane \( T_pS \) as will see next.

### 5.3.2 Morse lemma revisited and Dupin indicatrix

It is possible to have a local expression of any smooth function \( f(s,\lambda) \) around its non degenerate critical points in terms of the principal curvatures at \( p \). This is obtained by Taylor expanding \( f \) at \( p \) and then rotating the \( s\lambda \)-axes to coincide with the principal directions \( e_1 \) and \( e_2 \).

**Lemma 2 (Morse lemma revisited)** For each non degenerate critical point \( p \) of \( f \), there exists a neighbourhood of \( p \) such that

\[
f(\xi,\eta) = f(p) + \frac{1}{2} (k_1(p)\xi^2 + k_2(p)\eta^2) + \text{h.o.t.} \tag{5.5}
\]

with \( k_1(p) \) and \( k_2(p) \) are the principal curvatures of \( S \) at \( p \).

Let \( a > 0 \) be a positive small number. Dupin indicatrix is the set of vectors \( w \) in \( T_pS \) such that

\[
\Pi_p(w) = \pm a, \tag{5.6}
\]

with \( \Pi_p(w) = \langle du(p)(w), w \rangle \) the second fundamental form, which when expanded with \( w = \xi e_1 + \eta e_2 \), gives \( k_1(p)\xi^2 + k_2(p)\eta^2 \); hence, Dupin indicatrix is a union of conics in \( T_pS \). Lemma 2 says that, if \( p \) is a non degenerate critical point, the intersection with \( S \) of a plane parallel to \( T_pS \) is, in a first order approximation, a curve similar to (one of the conics of) the Dupin indicatrix at \( p \).

### 5.3.3 Delay factors around saddle points

Suppose now that the surface \( S \) is the graph of the function \( f(s,\lambda) = \det(H(s) - \lambda) \). By Lemma 2, if \( p \) is a non degenerate critical point of \( f \), then the spectrum of \( H(s) - \lambda \) given by the curve \( \{f(s,\lambda) = 0\} \) can be approximated by the Dupin indicatrix \( \{w = (\xi,\eta) \in \mathbb{R}^2 : \Pi_p(w) = -f(p)\} \), for some rotation \((s,\lambda) \mapsto (\xi,\eta)\). In particular, if \( p \) is a saddle point (i.e., \( k_1(p)k_2(p) < 0 \)), then the spectrum around \( p \) is a set of two hyperbola similar to those in the search problem discussed in the Introduction. In particular, the radius of Dupin indicatrix gives the energy difference, which in turn gives the total delay factor.

### 5.3.4 Tracking the shape operator

In light of the above, the shape operator \( d(n)(-\cdot) \) emerges as a central object in analyzing the computation advantage of AQC. Therefore, it is meaningful to connect the different locally defined shape operators around the different critical points consistently with the Morse complex; that is, to restrict the shape operator \( d(n)(-\cdot) \) to the network \( \mathcal{N} \subset S \) consisting of the critical points and the connecting instantons. By doing so, we obtain a fiber bundle (a subbundle of the tangent bundle \( TS \))

\[
\pi : \bigcup_{p \in \mathcal{N}} \{w \in T_pS : \Pi_p(w) = -f(p)\} \to \mathcal{N} \tag{5.7}
\]

that captures the adiabatic evolution of Hamiltonian \( H(s) \) not only topologically but also quantitatively around its critical points – at any saddle point \( p \in \mathcal{N} \) the total time delay...
can be obtained from the Dupin indicatrix. In fact, at the vicinity of any critical point \( p \), the spectrum of the time dependent Hamiltonian \( H(s) \) is completely determined (up to a rotation) by the spectrum of the hermitian operator \( d_n(p) \) acting on the 2-dimensional Hilbert space \( \mathbb{R}^2 \).

6 The Degenerate Case: Conley Theory

We summarize here relevant results from Conley theory—although there is no meaningful Hamiltonian of interest at this time. In Conley’s view, critical points of the function \( f \) are represented by the so-called index-pair which we review now – The following definitions and theorem are taken from [19]. A compact set \( N \subset M \) is said to be an isolating neighborhood of the flow \( \Phi_- \), if the set \( \text{Inv}(N, \Phi_-) = \{ x \in M | \Phi_{\tau}(x) \in N \text{ for all } \tau \in \mathbb{R} \} \) is contained in the interior of \( N \). An invariant set \( S \) is an isolated invariant set if there exists an isolating neighborhood \( N \) such that \( \text{Inv}(N, \Phi_-) = S \). Given an isolated invariant set \( S \), an index pair is a pair \( (N, L) \) where \( N \) is an isolating neighborhood, and \( L \) is an exit set – Figure 6.

Figure 6: (Left) An index pair for the saddle point \( p \). (Right) The Conley index is the homotopy type of the sphere obtained by collapsing \( L \) to a point (Images by T.O. Rot).

**Theorem 4 (C. Conley)** Let \( S \) be an isolated invariant set of the flow \( \Phi_- \). Then

- The set \( S \) admits an index pair \( (N, L) \).
- The Conley index is the pointed homotopy type \( (N \setminus L, [L]) \), and is independent of the choice of index pair.
- For any homotopy of flows \( \Phi_{\mu} \) (with \( \mu \in [0,1] \)) such that \( N \) is an isolating neighbourhood for all flows \( \Phi_{\mu} \), the Conley index of \( \text{Inv}(N, \Phi_-) \) remain unchanged for all \( \mu \).

An interesting case is the case of \( k \)-fold saddles which are the “degenerate analogue” of saddle points. Precisely, a \( k \)-fold saddle is a critical point at which \( f \) is locally given by \( \Re(e((x+iy))^{k+1}) \) with \( x, y \in \mathbb{R} \). An example is depicted in Figure 7. The function \( f(x, y) = x^3 - 3xy^2 \), which can be a characteristic function of some Hamiltonian \( H \), is perturbed into the Morse function \( f_\varepsilon(x, y) = x^3 - 3xy^2 + \varepsilon x \). The degenerate critical points bifurcates into two saddle points without affecting the dynamics around, and the results presented in the non degenerate case, can be extended to this type of degeneracy.

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7 Conclusion

In this paper we have presented a topological (qualitative) and geometrical (quantitative) description of the quantum adiabatic evolution for finite dimensional Hamiltonians. The topological description, based on gradient flows and Morse homology, gives the global picture of the evolution: critical points and how they connect to each other. The differential geometry description uses Gauß-Bonnet to zoom in, consistently with the topology, around the critical points to obtain the delay factors in the quantum adiabatic evolution. This global-to-local procedure can potentially serve as the foundation for a practical tool for designing efficient Hamiltonians for adiabatic quantum computations.

It is comforting, remarkable and, appealing, to see that the mathematics we have employed fit naturally with the physics. At the same time, many questions, that go beyond this connection, remain. For instance, can (physically motivated) Lyapunov functions be used? Is there a meaningful Hamiltonian where Conley theory is relevant? It is our modest hope that our approach opens up new avenues for studying quantum speedup in adiabatic quantum computations.

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