



Niall, Fintan, Shane

Applied Quantum Mechanics

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Adiabatic Theorem and Quantum Annealing

A Mathematically Rigorous Treatment

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- 3 Derivation of the Adiabatic Theorem
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The beginning of quantum theory

Einstein 1911 gave Solvay Conference on quantum hypothesis $E = nh\nu$ for atomic oscillators.

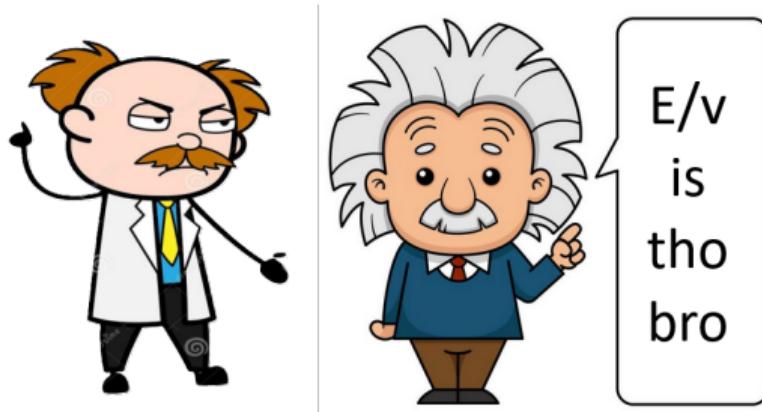


Figure: Einstein Lorentz Debate Cartoon Vecteezy



Figure: 1911 Solvay Conference Wikimedia Commons

Classical Analogy

A pendulum whose length changes slowly will maintain its oscillation mode, but if changed rapidly, it will exhibit chaotic behavior.

Also called adiabatic invariant, written by Ehrenfest in 1916 [4], and extended to quantum mechanics by Born and Fock in 1928 [3].

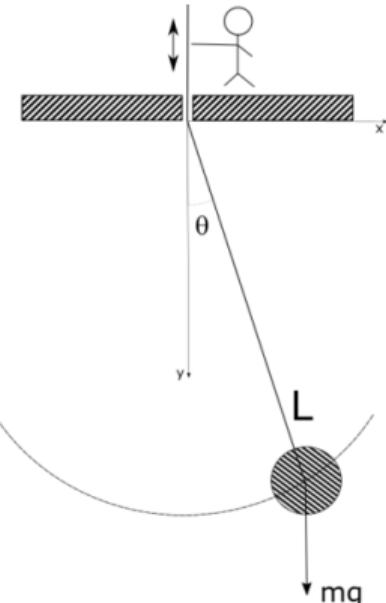


Figure: Pendulum with Varying Length
Wikimedia Commons

Physical Statement

If a quantum system starts in an eigenstate of a time-dependent Hamiltonian, and if the Hamiltonian changes **sufficiently slowly**, the system will remain in the corresponding instantaneous eigenstate throughout the evolution.

Figure: Slow change (animated)

- Key word: “**sufficiently slowly**”
- The system acquires a **dynamical phase** and a **geometric phase** (Berry phase)
- Fundamental to quantum computing (adiabatic quantum computation)
- Applies to quantum chemistry, biology / condensed matter physics

Figure: Abrupt change (animated)

Time-Dependent Schrödinger Equation

Consider a time-dependent Hamiltonian $\hat{H}(t)$:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle \quad (1)$$

Instantaneous Eigenstates

At each time t , we can solve the eigenvalue problem:

$$\hat{H}(t) |n(t)\rangle = E_n(t) |n(t)\rangle \quad (2)$$

where $|n(t)\rangle$ are the **instantaneous eigenstates** and $E_n(t)$ are the **instantaneous eigenvalues**.

Note: These are *not* solutions to the time-dependent Schrödinger equation, but rather eigenstates at fixed time t .

Substituting into Schrödinger Equation

Substitute the expansion $|\psi(t)\rangle = \sum_n c_n(t) e^{i\theta_n(t)} |n(t)\rangle$ into the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle$$
$$i\hbar \sum_n \left[\dot{c}_n e^{i\theta_n} |n\rangle + c_n i\dot{\theta}_n e^{i\theta_n} |n\rangle + c_n e^{i\theta_n} |\dot{n}\rangle \right] = \sum_n c_n e^{i\theta_n} E_n(t) |n\rangle \quad (3)$$

Dividing by $i\hbar$:

$$\sum_n \left[\frac{\dot{c}_n}{i\hbar} e^{i\theta_n} |n\rangle - \frac{c_n \dot{\theta}_n}{\hbar} e^{i\theta_n} |n\rangle + \frac{c_n}{i\hbar} e^{i\theta_n} |\dot{n}\rangle \right] = \sum_n \frac{c_n E_n}{i\hbar} e^{i\theta_n} |n\rangle \quad (4)$$

Projecting onto Eigenstates

Take the inner product with $\langle m(t)|$:

$$\frac{\dot{c}_m}{i\hbar}e^{i\theta_m} - \frac{c_m\dot{\theta}_m}{\hbar}e^{i\theta_m} + \frac{c_m}{i\hbar}e^{i\theta_m}\langle m|\dot{m}\rangle = \frac{c_mE_m}{i\hbar}e^{i\theta_m} \quad (5)$$

We used orthonormality: $\langle m|n\rangle = \delta_{mn}$ so that $\langle m|\hat{H}|n\rangle = E_m\delta_{mn}$.

Multiplying by $i\hbar$ and rearranging:

$$\dot{c}_m e^{i\theta_m} = c_m e^{i\theta_m} \left[i\hbar\dot{\theta}_m - E_m + i\hbar\langle m|\dot{m}\rangle \right] - \sum_{n \neq m} c_n e^{i\theta_n} \langle m|\dot{n}\rangle \quad (6)$$

Dynamical Phase

$$\theta_m(t) = -\frac{1}{\hbar} \int_0^t E_m(t') dt' + \gamma_m(t) \quad (7)$$

where $\gamma_m(t)$ is the **geometric phase** (Berry phase):

Geometric Phase

$$\gamma_m(t) = i \int_0^t \langle m(t') | \dot{m}(t') \rangle dt' \quad (8)$$

Then: $\dot{\theta}_m = -\frac{E_m}{\hbar} + i \langle m | \dot{m} \rangle$

Substituting back: $i\hbar \dot{\theta}_m - E_m + i\hbar \langle m | \dot{m} \rangle = 0$, so:

$$\dot{c}_m e^{i\theta_m} = - \sum_{n \neq m} c_n e^{i\theta_n} \langle m | \dot{n} \rangle \quad (9)$$



Figure: Michael Berry Wikimedia Commons

From the eigenvalue equation $\hat{H}(t)|n(t)\rangle = E_n(t)|n(t)\rangle$, differentiate with respect to t :

$$\dot{\hat{H}}|n\rangle + \hat{H}|\dot{n}\rangle = \dot{E}_n|n\rangle + E_n|\dot{n}\rangle \quad (10)$$

Take inner product with $\langle m|$ (where $m \neq n$):

$$\langle m| \dot{\hat{H}}|n\rangle + \langle m| \hat{H}|\dot{n}\rangle = \dot{E}_n \langle m|n\rangle + E_n \langle m|\dot{n}\rangle \quad (11)$$

Since $\langle m| \hat{H} = E_m \langle m|$ and $\langle m|n\rangle = 0$ for $m \neq n$:

$$\langle m| \dot{\hat{H}}|n\rangle + E_m \langle m|\dot{n}\rangle = E_n \langle m|\dot{n}\rangle \quad (12)$$

Matrix Element

$$\langle m|\dot{n}\rangle = \frac{\langle m| \dot{\hat{H}}|n\rangle}{E_n - E_m} \quad (m \neq n) \quad (13)$$

For the system to remain in state $|m\rangle$, we need $\dot{c}_m \approx 0$ for m equal to the initial state.

Adiabatic Condition

The Hamiltonian changes slowly enough that:

$$\left| \frac{\langle m | \dot{H} | n \rangle}{E_n - E_m} \right| \ll \frac{|E_n - E_m|}{\hbar} \quad (14)$$

for all $n \neq m$.

This can be rewritten as:

$$\left| \langle m | \dot{H} | n \rangle \right| \ll \frac{(E_n - E_m)^2}{\hbar} \quad (15)$$

Physical Interpretation: The time scale of Hamiltonian variation must be much larger than $\hbar/\Delta E$, where ΔE is the relevant energy gap.

Theorem (Quantum Adiabatic Theorem)

Let $\hat{H}(t)$ be a time-dependent Hamiltonian with instantaneous eigenstates $|n(t)\rangle$ and eigenvalues $E_n(t)$. Suppose:

- 1 The system starts in eigenstate $|n(0)\rangle$: $|\psi(0)\rangle = |n(0)\rangle$
- 2 The eigenvalues are non-degenerate
- 3 The adiabatic condition is satisfied for all $t \in [0, T]$

Then the state at time t is [7, 6]:

$$|\psi(t)\rangle = e^{i\theta_n(t)} |n(t)\rangle + \mathcal{O}(\epsilon) \quad (16)$$

where ϵ characterizes the adiabatic parameter and

$$\theta_n(t) = -\frac{1}{\hbar} \int_0^t E_n(t') dt' + i \int_0^t \langle n(t') | \partial_{t'} n(t') \rangle dt' \quad (17)$$

Example 1: Spin-1/2 in Rotating Magnetic Field

Consider a spin-1/2 particle in a magnetic field that rotates slowly:

$$\vec{B}(t) = B_0(\sin \theta \cos \omega t, \sin \theta \sin \omega t, \cos \theta) \quad (18)$$

The Hamiltonian is:

$$\hat{H}(t) = -\gamma \vec{B}(t) \cdot \vec{\sigma} = -\gamma B_0 \begin{pmatrix} \cos \theta & \sin \theta e^{-i\omega t} \\ \sin \theta e^{i\omega t} & -\cos \theta \end{pmatrix} \quad (19)$$

Instantaneous eigenvalues: $E_{\pm} = \mp \gamma B_0$

If the spin starts aligned with $\vec{B}(0)$ and ω is small enough:

- › The spin remains aligned with $\vec{B}(t)$ (adiabatic following)
- › After one full rotation ($t = 2\pi/\omega$), acquires Berry phase:
 $\gamma = \pi(1 - \cos \theta)$

Example 2: Two-Level System (Landau-Zener Model) [8, 11]

Consider the Landau-Zener Hamiltonian:

$$\hat{H}(t) = -\Delta\sigma_x - \epsilon(t)\sigma_z \quad (20)$$

where $\epsilon(t)$ is swept linearly from $\epsilon_i < 0$ to $\epsilon_f > 0$.

Energy eigenvalues:

$$E_{\pm}(t) = \pm\sqrt{\Delta^2 + \epsilon^2(t)} \quad (21)$$

Energy gap at crossing ($\epsilon = 0$):

$$\Delta E_{\min} = 2\Delta$$

Figure: Landau-Zener dynamics (animated)

For a cyclic adiabatic evolution, where the Hamiltonian returns to its initial form:

$$\hat{H}(R(T)) = \hat{H}(R(0)) \quad (22)$$

The total phase acquired is:

$$e^{i\phi} = e^{i\theta_{\text{dyn}}} e^{i\gamma_n} \quad (23)$$

Berry Phase (1984) [2]

$$\gamma_n = i \oint_{\mathcal{C}} \langle n(R) | \nabla_R n(R) \rangle \cdot dR \quad (24)$$

where \mathcal{C} is the closed path in parameter space.

Properties:

- Gauge invariant (physical observable)
- Geometric: depends only on path, not speed
- Can be written as flux of Berry curvature

Berry Connection (Vector Potential)

$$\vec{A}_n(R) = i \langle n(R) | \nabla_R n(R) \rangle \quad (25)$$

Berry Curvature (Field Strength)

$$\vec{F}_n(R) = \nabla_R \times \vec{A}_n(R) \quad (26)$$

By Stokes' theorem:

$$\gamma_n = \oint_C \vec{A}_n \cdot dR = \iint_S \vec{F}_n \cdot d\vec{S} \quad (27)$$

Analogy: Berry phase is like the Aharonov-Bohm phase, but in parameter space rather than real space!

When adiabaticity breaks down, transitions occur between energy levels.

Landau-Zener Formula

For a linear crossing: $E_1(t) = \alpha t$, $E_2(t) = -\alpha t + \Delta$

Transition probability:

$$P_{1 \rightarrow 2} = \exp\left(-\frac{\pi\Delta^2}{2\hbar\alpha}\right) \quad (28)$$

- Small gap $\Delta \Rightarrow$ high transition probability
- Fast sweep (large α) \Rightarrow high transition probability
- Slow sweep (small α) \Rightarrow adiabatic regime, $P \rightarrow 0$

We can systematically expand in the adiabatic parameter $\epsilon = \tau_{\text{dyn}}/T$:

$$|\psi(t)\rangle = e^{i\theta_n(t)} \left[|n(t)\rangle + \epsilon |\psi_n^{(1)}(t)\rangle + \epsilon^2 |\psi_n^{(2)}(t)\rangle + \dots \right] \quad (29)$$

First-order correction:

$$|\psi_n^{(1)}(t)\rangle = \sum_{m \neq n} \frac{\langle m | \dot{\hat{H}} | n \rangle}{(E_n - E_m)^2} |m\rangle \quad (30)$$

This shows:

- › Transition amplitude $\propto 1/(E_n - E_m)^2$
- › Small gaps make adiabatic evolution difficult
- › Can estimate fidelity: $|\langle n(t) | \psi(t) \rangle|^2 \approx 1 - \mathcal{O}(\epsilon^2)$

When eigenvalues are degenerate, the theorem must be modified:

- › System can transition within degenerate subspace
- › Need to consider the entire degenerate subspace
- › Berry phase becomes a **matrix** (non-Abelian Berry connection)

Wilczek-Zee Connection [10]

For degenerate subspace with basis $\{|n_a(R)\rangle\}$:

$$(A_i)_{ab} = i \langle n_a | \partial_i n_b \rangle \quad (31)$$

This is a matrix-valued gauge potential.

Leads to non-Abelian geometric phases (important in topological quantum computation).

Application: Adiabatic Quantum Computation [5, 1]

$$\hat{H}(t) = (1 - s(t))\hat{H}_{\text{initial}} + s(t)\hat{H}_{\text{problem}} \quad (32)$$

Basic Idea

- 1 Encode problem in Hamiltonian \hat{H}_{problem} whose ground state is the solution
- 2 Start with simple Hamiltonian \hat{H}_{initial} with known ground state
- 3 Slowly interpolate: $\hat{H}(t) = (1 - s(t))\hat{H}_{\text{initial}} + s(t)\hat{H}_{\text{problem}}$
- 4 If evolution is adiabatic, system remains in ground state
- 5 At $t = T$: measure to obtain solution

Runtime: $T \sim \mathcal{O}(\hbar/\Delta_{\min}^2)$ where Δ_{\min} is minimum gap

Challenge: Gap can be exponentially small for some problems!

Adiabatic Theorem in Quantum Annealing

Success condition based on adiabatic theorem:

Required Annealing Time

$$T \gg \frac{\hbar}{\Delta_{\min}^2} \quad (33)$$

where Δ_{\min} is the minimum energy gap during evolution

Problem-Dependent Gap:

- Different problems \Rightarrow different gap structures
- Gap often smallest near $t \approx T/2$ (mid-anneal)
- For many NP-hard problems: $\Delta_{\min} \sim e^{-\alpha N}$ (exponentially small!)

Practical Implications:

- + Easy problems: Fast annealing possible (microseconds)
- Hard problems: May need exponentially long annealing time
- ± Thermal effects can help/hinder (quantum vs simulated annealing)

Goal: Solve optimization problems using quantum adiabatic evolution

Standard Approach

- 1 Encode optimization problem in a Hamiltonian
- 2 Prepare system in ground state of simple initial Hamiltonian
- 3 Adiabatically evolve to problem Hamiltonian
- 4 Measure final state to read out solution

Two Main Formulations:

- **Ising Model:** Spin variables $s_i \in \{-1, +1\}$
- **QUBO:** Binary variables $x_i \in \{0, 1\}$
- These are equivalent and interconvertible

Examples: Graph coloring, traveling salesman, portfolio optimization, protein folding [9]

Ising Hamiltonian

$$\hat{H}_{\text{Ising}} = \sum_{i < j} J_{ij} s_i s_j + \sum_i h_i s_i \quad (34)$$

where $s_i \in \{-1, +1\}$ are spin variables (Pauli-z eigenvalues)

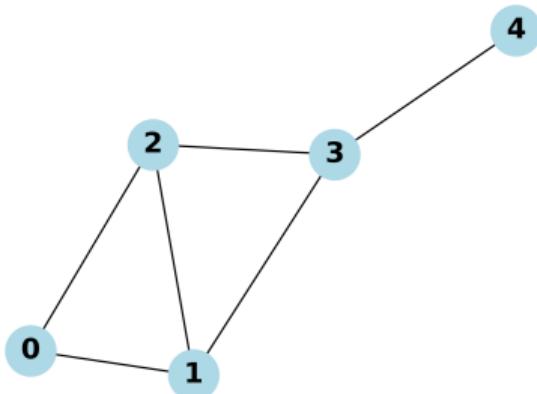
Parameters:

- J_{ij} : Coupling between spins i and j
 - » $J_{ij} > 0$: Ferromagnetic (spins want to align)
 - » $J_{ij} < 0$: Antiferromagnetic (spins want to anti-align)
- h_i : Local field on spin i (bias)

This is the **problem Hamiltonian** in quantum annealing!

Visualizing the Ising Model: Max-Cut Example

Example Graph for Max-Cut



Optimal Max-Cut (size = 5)

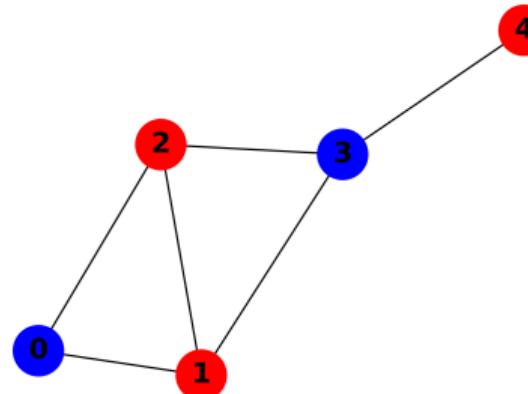


Figure: Max-Cut example graph (problem instance)

- **Left:** Original graph with 5 vertices and 6 edges
- **Right:** Optimal partition (red vs blue) achieves cut size = 5
- Only 1 edge (out of 6) remains within a partition
- Ising formulation: Antiferromagnetic couplings ($J_{ij} = 1$) favor opposite spins

QUBO: Quadratic Unconstrained Binary Optimization

QUBO Formulation

Minimize:

$$f(x) = \sum_i Q_{ii}x_i + \sum_{i < j} Q_{ij}x_i x_j = x^T Q x \quad (35)$$

where $x_i \in \{0, 1\}$ and Q is the QUBO matrix

Why QUBO?

- Many combinatorial optimization problems naturally expressed as QUBO
- NP-hard in general (finding global minimum)
- Can encode constraints via penalty terms

Examples:

- Max-Cut: $\max \sum_{(i,j) \in E} (1 - x_i x_j)$
- Number Partitioning: $\min (\sum_i a_i x_i)^2$
- Graph Coloring: Use penalty for adjacent same-colored vertices

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