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Applied Quantum Mechanics

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Adiabatic Theorem and Quantum Annealing

A Mathematically Rigorous Treatment

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The beginning of quantum theory

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

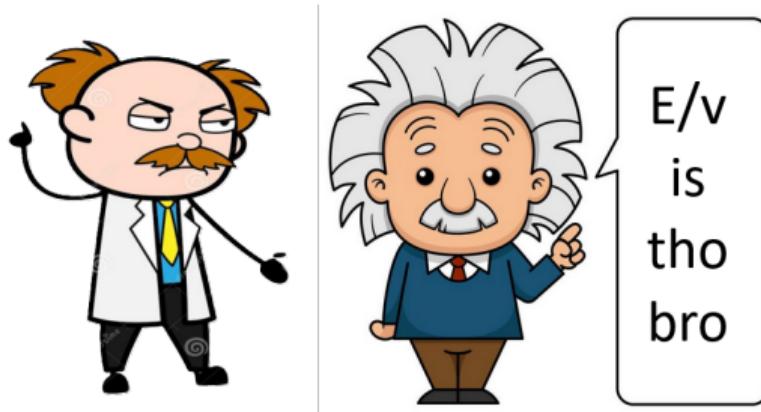


Figure: Einstein Lorentz Debate Cartoon Vecteezy



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, and extended to quantum mechanics by Born and Fock in 1928.

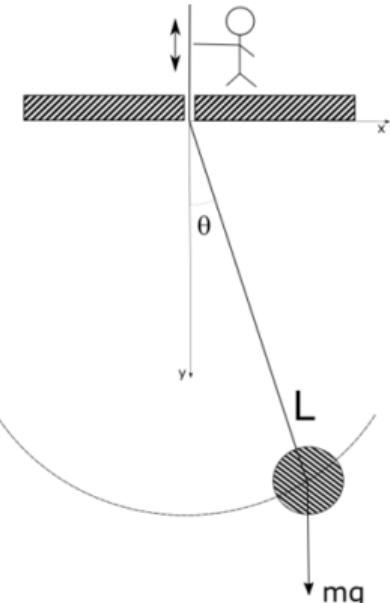


Figure: Pendulum with Varying Length
Wikimedia Commons

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:

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

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)

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)

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

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

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

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

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

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)

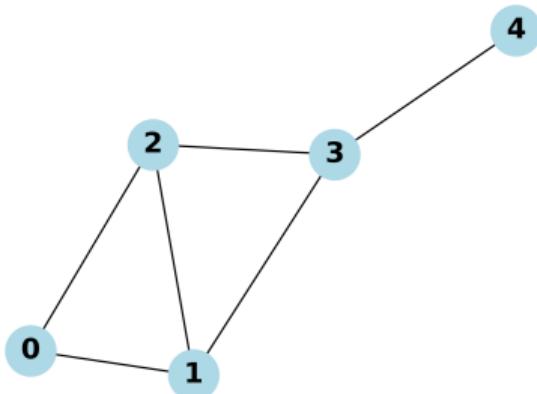
Parameters:

- 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)

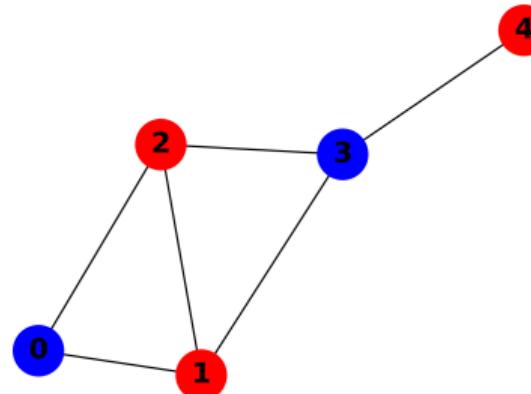


Figure: Max-Cut example graph (problem instance)

- **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

Born-Oppenheimer Approximation: Adiabatic Physics in Molecules

$$\Psi(\mathbf{r}, \mathbf{R}) \approx \psi_e(\mathbf{r}; \mathbf{R}) \chi(\mathbf{R})$$

- **Separation of timescales:** Nuclei (heavy) move slowly, electrons adapt instantaneously.
- The electronic Hamiltonian $H_e(\mathbf{R})$ depends *parametrically* on the nuclear coordinates.
- By the **adiabatic theorem**, the electronic state remains in the instantaneous ground state as nuclei evolve slowly.

Analogy to Adiabatic Quantum Computing

Slow nuclear motion \leftrightarrow slow Hamiltonian evolution. Electrons follow adiabatically \leftrightarrow qubit states follow instantaneous ground state.

Thank You!

Questions?

Appendix: Why instantaneous eigenstates are not TDSE solutions

Suppose the instantaneous eigenproblem holds:

$$\hat{H}(t) |n(t)\rangle = E_n(t) |n(t)\rangle. \quad (36)$$

Ask whether $|\psi(t)\rangle = e^{i\theta(t)} |n(t)\rangle$ can satisfy the time-dependent Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H}(t) |\psi(t)\rangle. \quad (37)$$

Plugging in gives:

$$i\hbar \left(\dot{\theta} |n\rangle + |\dot{n}\rangle \right) = E_n |n\rangle. \quad (38)$$

Project onto an orthogonal eigenstate $\langle m(t)|$ with $m \neq n$ to obtain the consistency condition:

$$i\hbar \langle m | \dot{n} \rangle = 0 \quad (m \neq n). \quad (39)$$

But differentiating the eigenvalue equation and projecting onto $\langle m|$ yields

$$\langle m | \dot{n} \rangle = \frac{\langle m | \dot{\hat{H}} | n \rangle}{E_n - E_m} \quad (m \neq n), \quad (40)$$

i/iv

Appendix: Proof of $\langle n|\dot{n} \rangle$ is Purely Imaginary

From normalization: $\langle n|n \rangle = 1$

Differentiate with respect to time:

$$\frac{d}{dt} \langle n|n \rangle = \langle \dot{n}|n \rangle + \langle n|\dot{n} \rangle = 0 \quad (41)$$

Therefore:

$$\langle n|\dot{n} \rangle = -\langle \dot{n}|n \rangle = -\langle n|\dot{n} \rangle^* \quad (42)$$

This implies $\langle n|\dot{n} \rangle$ is purely imaginary.

We can write: $\langle n|\dot{n} \rangle = i\gamma_n(t)$ where $\gamma_n(t)$ is real.

Appendix: Derivation of Berry Curvature

Starting from Berry connection:

$$A_i = i \langle n | \partial_i n \rangle \quad (43)$$

The Berry curvature is:

$$F_{ij} = \partial_i A_j - \partial_j A_i \quad (44)$$

Expanding:

$$F_{ij} = i [\partial_i \langle n | \partial_j n \rangle - \partial_j \langle n | \partial_i n \rangle] \quad (45)$$

$$= i [\langle \partial_i n | \partial_j n \rangle + \langle n | \partial_i \partial_j n \rangle - \langle \partial_j n | \partial_i n \rangle - \langle n | \partial_j \partial_i n \rangle] \quad (46)$$

Since $\partial_i \partial_j = \partial_j \partial_i$:

$$F_{ij} = i [\langle \partial_i n | \partial_j n \rangle - \langle \partial_j n | \partial_i n \rangle] \quad (47)$$

Appendix: Completeness Relation

Using completeness: $\sum_m |m\rangle \langle m| = \mathbb{I}$

We can write:

$$|\partial_i n\rangle = \sum_m |m\rangle \langle m| \partial_i n \rangle \quad (48)$$

Therefore:

$$\langle \partial_i n | \partial_j n \rangle = \sum_{m,k} \langle \partial_i n | k \rangle \langle k | m \rangle \langle m | \partial_j n \rangle \quad (49)$$

$$= \sum_m \langle \partial_i n | m \rangle \langle m | \partial_j n \rangle \quad (50)$$

The Berry curvature becomes:

$$F_{ij} = i \sum_{m \neq n} [\langle \partial_i n | m \rangle \langle m | \partial_j n \rangle - \langle \partial_j n | m \rangle \langle m | \partial_i n \rangle] \quad (51)$$