A Note on the Adiabatic Theorem of Quantum Mechanics[*]

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The adiabatic theorem in quantum theory refers to a situation in which the original Hamiltonian of a system is gradually changed into a new Hamiltonian. Roughly speaking, the theorem states that an eigenstate for the original energy becomes approximately an eigenstate for the new energy if the switch-on of the energy difference is sufficiently slow.

The model for this situation is given by a time-dependent Schrödinger equation with slowness parameter $\epsilon \ll 1$,

$$i\dot{\psi}_\epsilon = H(\epsilon t)\psi_\epsilon, \qquad \psi_\epsilon(0) = \psi_*.$$

The switch-on of the change takes place at time $t_0 = 0$, the switch-off at time $t_1 = T/\epsilon$. We are interested in the limit situation $\epsilon \to 0$ of an "infinitely slow" change. It is convenient to transform the time variable linearly onto the fixed interval $[0, T]$, yielding the singularly perturbed equation

$$i\epsilon\dot{\psi}_\epsilon = H(t)\psi_\epsilon, \qquad \psi_\epsilon(0) = \psi_*. \tag{1}$$

We will address the *finite dimensional* setting $\psi(t) \in \mathbb{C}^d$ by using perturbation theory of integrable Hamiltonian systems.

The key point is to observe that the time-dependent Schrödinger equation has a canonical structure. To this end, we use phase-space coordinates $(i\epsilon\,\psi_\epsilon, \psi_\epsilon^\dagger; E_\epsilon, t)$, with time t being the canonical momentum corresponding to the *energy* E_ϵ, the symplectic two-form

$$\sigma = i\epsilon\, d\psi_\epsilon \wedge d\psi_\epsilon^\dagger + dE_\epsilon \wedge dt$$

and the Hamiltonian function[‡]

$$\mathscr{Z} = \langle H(t)\psi_\epsilon, \psi_\epsilon\rangle - E_\epsilon.$$

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[‡] To get an *autonomous* system

In fact, using Wirtinger derivatives, the Schrödinger equation Eq. (1) is equivalent to *both* of the equations[§]

$$i\epsilon\dot{\psi}_\epsilon = \frac{\partial \mathcal{Z}}{\partial \psi_\epsilon^\dagger}, \qquad \dot{\psi}_\epsilon^\dagger = -\frac{1}{i\epsilon}\frac{\partial \mathcal{Z}}{\partial \psi_\epsilon}.$$

The other two canonical equations are just

$$\dot{E}_\epsilon = \frac{\partial \mathcal{Z}}{\partial t} = \langle \dot{H}(t)\psi_\epsilon, \psi_\epsilon\rangle, \qquad \dot{t} = -\frac{\partial \mathcal{Z}}{\partial E_\epsilon} = 1.$$

We choose the additional initial values

$$E_\epsilon(0) = E_* = \langle H(0)\psi_*, \psi_*\rangle, \qquad t_* = 0.$$

Hence, the value of the invariant of motion $\mathcal{Z}$ is fixed to be *zero.*[¶]. We will assume right from the beginning that all eigenvalues $\omega_\lambda(t)$ of the d-dimensional hermitian matrix $H(t)$ are simple and that there are no resonances of order two,

$$\omega_\lambda(t) \neq \omega_\mu(t), \qquad t \in \mathbb{R},\ \lambda \neq \mu.$$

There is a family of orthonormal eigenvectors $(e_1(y), \ldots, e_r(y))$,

$$H(y)e_\lambda(y) = \omega_\lambda(y)e_\lambda(y), \qquad \langle e_\lambda(y), e_\mu(y)\rangle = \delta_{\lambda\mu}.$$

This normalization yields an important anti-hermitian relation of the time-derivatives $\dot{e}_\lambda$, specifically

$$\langle e_\lambda, \dot{e}_\mu\rangle = -\langle e_\mu, \dot{e}_\lambda\rangle^\dagger. \tag{2}$$

We introduce particular action-angle variables $(\theta_\epsilon, \phi_\epsilon)$,

$$\psi_\epsilon = \sum_\lambda \sqrt{\theta_\epsilon^\lambda}\exp(-i\epsilon^{-1}\phi_\epsilon^\lambda)\, e_\lambda.$$

This transformation yields the one-form

$$d\psi_\epsilon = \sum_\lambda \sqrt{\theta_\epsilon^\lambda}\exp(-i\epsilon^{-1}\phi_\epsilon^\lambda)\left(-i\epsilon^{-1}e_\lambda\, d\phi_\epsilon^\lambda + \frac{1}{2\theta_\epsilon^\lambda}e_\lambda\, d\theta_\epsilon^\lambda + \dot{e}_\lambda\, dt\right).$$

Hence, by using the normalization $\langle e_\lambda, e_\mu\rangle = \delta_{\lambda\mu}$ and the anti-hermitian relation Eq. (2), we obtain

$$\begin{aligned} i\epsilon\, d\psi_\epsilon \wedge d\psi_\epsilon^\dagger &= \sum_\lambda d\phi_\epsilon^\lambda \wedge d\theta_\epsilon^\lambda \\ &\quad + 2\sum_{\lambda,\mu}\sqrt{\theta_\epsilon^\lambda\theta_\epsilon^\mu}\,\Re\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right)\langle e_\lambda, \dot{e}_\mu\rangle\right)\, d\phi_\epsilon^\lambda \wedge dt \\ &\quad - \epsilon\sum_{\lambda,\mu}\sqrt{\frac{\theta_\epsilon^\mu}{\theta_\epsilon^\lambda}}\,\Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right)\langle e_\lambda, \dot{e}_\mu\rangle\right)\, d\theta_\epsilon^\lambda \wedge dt. \end{aligned}$$

[§] Thus, the real dimension of the phase space is effectively $2d + 2$, eliminating the duplication of information in using *both* ψ_ϵ and $\psi_\epsilon^\dagger$

[¶] Which explains the choice of the letter $\mathcal{Z}$

However, for obtaining a transformation being symplectic on the phase-space as a whole, we additionally have to transform the energy variable E_ϵ,

$$E_\epsilon = P_\epsilon + \epsilon \sum_{\lambda,\mu} \sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}\; \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right). \tag{3}$$

By the anti-hermitian relation Eq. (2), this transformation results in

$$\begin{aligned} dE_\epsilon \wedge dt &= dP_\epsilon \wedge dt \\ &\quad - 2\sum_{\lambda,\mu} \sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}\; \Re\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right)\, d\phi_\epsilon^\lambda \wedge dt \\ &\quad + \epsilon \sum_{\lambda,\mu} \sqrt{\frac{\theta_\epsilon^\mu}{\theta_\epsilon^\lambda}}\; \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right)\, d\theta_\epsilon^\lambda \wedge dt. \end{aligned}$$

Altogether, these lengthy but straightforward calculations have proven that the transformation $(\psi_\epsilon, \psi_\epsilon^\dagger; E_\epsilon, t) \mapsto (\phi_\epsilon, \theta_\epsilon; t, P_\epsilon)$ is symplectic indeed,

$$\sigma = i\epsilon\, d\psi_\epsilon \wedge d\psi_\epsilon^\dagger + dE_\epsilon \wedge dt = \sum_\lambda d\phi_\epsilon^\lambda \wedge d\theta_\epsilon^\lambda + dP_\epsilon \wedge dt.$$

The autonomous Hamiltonian function $\mathcal{Z}$ transforms to the expression

$$\mathcal{Z} = \sum_\lambda \theta_\epsilon^\lambda \cdot \omega_\lambda - P_\epsilon - \;\epsilon \sum_{\lambda,\mu} \sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}\; \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right).$$

Thus, by the canonical formalism, the equation of motion take the form

$$\dot{\phi}_\epsilon^\lambda = \frac{\partial \mathcal{Z}}{\partial \theta_\epsilon^\lambda}, \qquad \dot{\theta}_\epsilon^\lambda = -\frac{\partial \mathcal{Z}}{\partial \phi_\epsilon^\lambda}, \qquad \dot{P}_\epsilon = \frac{\partial \mathcal{Z}}{\partial t}, \qquad \dot{t} = -\frac{\partial \mathcal{Z}}{\partial P_\epsilon} = 1,$$

i.e., after some calculation,

$$\begin{aligned} \dot{\phi}_\epsilon^\lambda &= \omega_\lambda \;-\; \epsilon \sum_\mu \sqrt{\frac{\theta_\epsilon^\mu}{\theta_\epsilon^\lambda}}\; \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right) \\ \dot{\theta}_\epsilon^\lambda &= \;-2\sum_{\mu\neq\lambda} \sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}\; \Re\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \langle e_\lambda, \dot{e}_\mu\rangle\right) \\ \dot{P}_\epsilon &= \sum_\lambda \theta_\epsilon^\lambda \cdot \dot{\omega}_\lambda \\ &\quad - \epsilon \sum_{\lambda\mu} \sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}\; \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right) \left(\langle \dot{e}_\lambda, \dot{e}_\mu\rangle + \langle e_\lambda, \ddot{e}_\mu\rangle\right)\right). \end{aligned}$$

The initial values transform as follows. Using polar coordinates,

$$\langle \psi_*, e_\lambda(0)\rangle = \sqrt{\theta_*^\lambda} \cdot \exp\left(-i\phi_*^\lambda\right), \qquad \lambda = 1, \ldots, r,$$

we obtain

$$\phi_\epsilon(0) = \epsilon\phi_*, \qquad \theta_\epsilon(0) = \theta_*, \qquad P_\epsilon(0) = E_* + O(\epsilon).$$

Now, for eliminating the fast dependence on the angle variables of the $O(1)$-terms we introduce the transformed action variables

$$\Theta_\epsilon^\lambda = \theta_\epsilon^\lambda - 2\epsilon \sum_{\mu\neq\lambda} \frac{\sqrt{\theta_\epsilon^\lambda \theta_\epsilon^\mu}}{\omega_\lambda - \omega_\mu}\, \Im\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right)\langle e_\lambda, \dot e_\mu\rangle\right), \qquad (4)$$

with initial value $\Theta_\epsilon(0) = \theta_* + O(\epsilon)$. Since we have excluded any resonance of order two, this transformation is well-defined. For Θ_ϵ the equation of motion takes the simple form

$$\dot\Theta_\epsilon = O(\epsilon),$$

yielding the estimate

$$\Theta_\epsilon = \theta_* + O(\epsilon), \qquad \text{i.e.,} \qquad \theta_\epsilon = \theta_* + O(\epsilon).$$

Thus, the energy level probabilities are *adiabatic invariants.* Likewise, elimination of the $O(\epsilon)$ term in the equations for ϕ_ϵ is achieved by introducing

$$\Phi_\epsilon^\lambda = \phi_\epsilon^\lambda + \epsilon^2 \sum_{\mu\neq\lambda} \frac{\sqrt{\theta_*^\mu/\theta_*^\lambda}}{\omega_\lambda - \omega_\mu}\, \Re\left(\exp\left(-i\epsilon^{-1}(\phi_\epsilon^\lambda - \phi_\epsilon^\mu)\right)\langle e_\lambda, e_\mu\rangle\right)$$

with initial value $\Phi_\epsilon(0) = \epsilon\phi_* + O(\epsilon^2)$. This transformation is only well-defined, if the energy level λ is initially excited, $\theta_*^\lambda \neq 0$. We denote the set of all these levels by Λ_{ex}. For $\lambda \in \Lambda_{\text{ex}}$ the equation of motion is now given by

$$\dot\Phi_\epsilon^\lambda = \omega_\lambda - \epsilon\,\Im\langle e_\lambda, \dot e_\lambda\rangle + O(\epsilon^2),$$

yielding the estimate

$$\phi_\epsilon^\lambda = \Phi_\epsilon^\lambda + O(\epsilon^2) = \phi_{\text{av}}^\lambda + \epsilon\phi_{\text{Berry}}^\lambda + O(\epsilon^2),$$

with

$$\phi_{\text{av}}^\lambda(t) = \int_0^t \omega_\lambda(\tau)\,d\tau, \qquad \phi_{\text{Berry}}^\lambda(t) = \phi_*^\lambda + i\int_0^t \langle e_\lambda(\tau), \dot e_\lambda(\tau)\rangle\,d\tau.$$

Notice, that because of the anti-hermitian relation Eq. (2) the term $\langle e_\lambda, \dot e_\lambda\rangle$ is purely *imaginary.* Altogether, we have obtained an order $O(\epsilon)$ approximation of the wave function ψ_ϵ itself,

$$\psi_\epsilon = \sum_{\lambda\in\Lambda_{\text{ex}}} \sqrt{\theta_*^\lambda}\,\exp(-i\phi_{\text{Berry}}^\lambda)\exp(-i\epsilon^{-1}\phi_{\text{av}}^\lambda)\,e_\lambda \;+\; O(\epsilon).$$

Finally, there is no difficulty left to prove the energy estimate

$$E_\epsilon = \sum_\lambda \theta_*^\lambda \cdot \omega_\lambda \;+\; O(\epsilon).$$

Remarks and Observations. We conclude by discussing some interesting points.

1. Using the new action-angle variables, the Hamiltonian function $\mathcal{Z}$ had to be expanded *including* the first order term in ϵ. Otherwise the *zero* order term of the equation for $\dot{\theta}_\epsilon$ would have been unknown and a proof of the adiabatic invariance of θ_ϵ would have been impossible.

2. Because of the factor ϵ^{-1} multiplying the angle ϕ_ϵ in the expression for the wavefunction ψ_ϵ we had to expand the angle up to an error of *second* order for obtaining a first order approximation of ψ.

3. The occurrence of the Berry-phase ϕ_{Berry} can be understood as making the zero-order approximation of the wave-function *gauge-invariant*, i.e., invariant with respect to a phase transformation of the eigenvectors
$$e_\lambda \mapsto \exp(i\gamma_\lambda)\, e_\lambda.$$

4. Using the method of stationary phase, one can prove that the given approximation of ψ_ϵ directly implies
$$\psi_\epsilon \overset{*}{\rightharpoonup} 0 \qquad \text{in} \quad L^\infty([0,T],\mathbb{C}^d),$$
provided the eigenvalue families ω_λ just have isolated zeroes.

5. Since there are no resonances, the method of stationary phase applied to the density matrix $\rho_\epsilon = \psi_\epsilon \psi_\epsilon^\dagger$ yields the weak limit
$$\rho_\epsilon \overset{*}{\rightharpoonup} \rho_0 = \sum_{\lambda\in\Lambda_{\mathrm{ex}}} \theta_*^\lambda \cdot e_\lambda e_\lambda^\dagger.$$