Title: A variety of results in mathematical adiabatic quantum mechanics

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Abstract:

A Variety of Mathematical Results in Adiabatic Quantum Mechanics

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The Simplest Situation for Adiabatic Quantum Mechanics

$$i\,\frac{d\phi}{ds} = H(\epsilon s)\,\phi, \qquad \text{for} \quad -T/\epsilon \le s \le T/\epsilon.$$

Rescale time by $t = \epsilon s$ to rewrite this as

$$i\,\epsilon\,\frac{d\psi}{dt} = H(t)\,\psi, \qquad \text{for} \quad -T \le t \le T.$$

Assume $H(t)$ is self-adjoint, depends smoothly on t, and has a multiplicity 1 eigenvalue $E(t)$ that depends continuously on t.

Further assume $H(t)$ satisfies the gap condition

$$\text{dist}\,\{\,E(t),\,\sigma(H(t))\backslash E(t)\,\} = g(t) \ge g_0 > 0 \quad \text{for} \quad -T \le t \le T.$$

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The Adiabatic Connection. We can choose a normalized eigenvector $\Phi(t)$ that corresponds to $E(t)$, depends smoothly on t, and satisfies

$$\langle \Phi(t), \dot{\Phi}(t) \rangle = 0.$$

In this sense, there are no Berry Phase issues when the eigenvector depends on only 1 parameter.
However, we might have $H(t_1) = H(t_2)$, but $\Phi(t_1) \neq \Phi(t_2)$.

Proof: By standard perturbation theory there exists a smooth, normalized choice $\Phi_1(t)$ of eigenvector corresponding to $E(t)$.

Since $0 = \frac{d}{dt} \|\Phi_1(t)\|^2 = \langle \Phi_1(t), \dot{\Phi}_1(t) \rangle + \langle \dot{\Phi}_1(t), \Phi_1(t) \rangle$,

$\langle \Phi_1(t), \dot{\Phi}_1(t) \rangle$ is purely imaginary.

So, $\theta(t) = \int_0^t i \langle \Phi_1(r), \dot{\Phi}_1(r) \rangle \, dr$ is real.

Simply verify that $\Phi(t) = e^{i\theta(t)} \Phi_1(t)$ satisfies the requirements.

$$\begin{pmatrix} \cos t & \sin t \\ \sin t & -\cos t \end{pmatrix}$$

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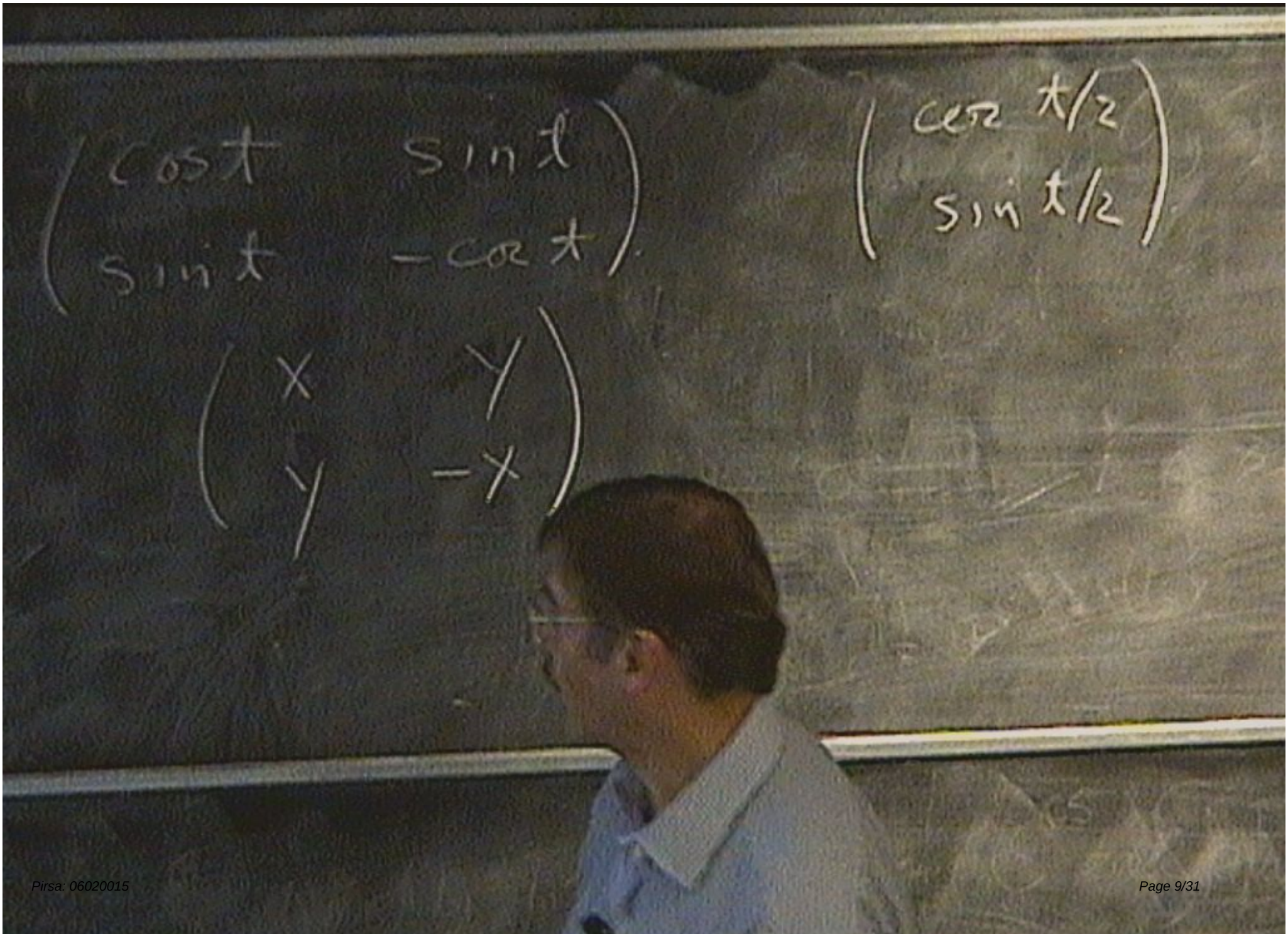
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Theorem 1. The Schrödinger equation has a solution of the form

$$e^{-i\int_0^t E(s)\,ds/\epsilon}\ \Phi(t) + O(\epsilon),$$

where the error term denotes the norm of the error.

This can be improved to the following:

Theorem 2. For any positive integer N, the Schrödinger equation has a solution of the form

$$e^{-i\int_0^t E(s)\,ds/\epsilon}\left[\Phi(t) + \epsilon\psi_1(t) + \epsilon^2\psi_2(t) + \cdots + \epsilon^N\psi_N(t)\right] + O(\epsilon^{N+1}).$$

There are two standard approaches for proving these results:

1. An integration by parts technique, due originally to Kato in 1949.

2. An asymptotic expansions technique, due originally to Born and Fock in 1928.

Remark If $H(t)$ is analytic in a complex neighborhood of the real interval $[-T, T]$, then optimal truncation of the asymptotic series yields an approximation with errors of order $\exp\left(-\frac{C}{\epsilon}\right)$.

Lemma. Suppose $\psi_\epsilon(t)$ is a smooth, vector-valued function. Define

$$\zeta_\epsilon(t) \;=\; i\,\epsilon\,\frac{d\psi_\epsilon}{dt}(t) \;-\; H(t)\;\psi_\epsilon(t).$$

If $\|\,\zeta_\epsilon(t)\,\| \;\leq\; \mu(\epsilon,\,t)$, then $\psi_\epsilon(t)$ agrees with an exact solution of the Schrödinger equation up to an error whose norm is bounded by

$$\frac{1}{\epsilon}\;\int_0^t \mu(\epsilon,\,s)\;ds.$$

Proof: Let $U_\epsilon(t,\,s)$ denote the propagator for the Schrödinger equation. The norm of the error is then

$$\begin{aligned}
&\|\;\psi_\epsilon(t) \;-\; U_\epsilon(t,\,0)\;\psi_\epsilon(0)\;\| \\
&= \;\|\;U_\epsilon(0,\,t)\;\psi_\epsilon(t) \;-\; \psi_\epsilon(0)\;\| \\
&= \;\left\|\;\int_0^t \frac{d}{ds}\,U_\epsilon(0,\,s)\;\psi_\epsilon(s)\;ds\;\right\| \\
&= \;\left\|\;\int_0^t U_\epsilon(0,\,s)\;\left(\,i\,H(s)\,\psi_\epsilon(s)/\epsilon \;-\; \frac{d\psi_\epsilon}{ds}(s)\,\right)\;ds\;\right\| \\
&\leq \;\frac{1}{\epsilon}\;\int_0^t \mu(\epsilon,\,s)\;ds.
\end{aligned}$$

Proofs of the Theorems: Make the Ansatz that the Schrödinger equation has a solution of the form

$$e^{-i\int_0^t E(s)\,ds/\epsilon}\left[\psi_0(t) + \epsilon\psi_1(t) + \epsilon^2\psi_2(t) + \cdots\right]$$

Substitute this into the Schrödinger equation to obtain

$$i\,\epsilon\left(\dot\psi_0(t) + \epsilon\dot\psi_1(t) + \epsilon\dot\psi_2(t) + \cdots\right)$$

$$= [H(t) - E(t)]\left(\psi_0(t) + \epsilon\psi_1(t) + \epsilon^2\psi_2(t) + \cdots\right).$$

Then simply equate terms of the same orders on the two sides of this equation.

Order 0. The order ϵ^0 terms require

$$[H(t) - E(t)]\,\psi_0(t) = 0.$$

Thus,

$$\psi_0(t) = f_0(t)\,\Phi(t),$$

where we do not yet have any information about $f_0(t)$.

Order 1. The order ϵ^1 terms require

$$i\,\dot f_0(t)\,\Phi(t) + i\,f_0(t)\,\dot\Phi(t) = [H(t) - E(t)]\,\psi_1(t).$$

The components of the two sides in the direction of $\Phi(t)$ must be equal, and the components orthogonal to $\Phi(t)$ must be equal.

Using our choice of phase for $\Phi(t)$, we obtain the two equations:

$$i\,\dot{f}_0(t) \;=\; 0.$$

$$[H(t) - E(t)]\;\psi_1(t) \;=\; i\,f_0(t)\,\dot{\Phi}(t).$$

From the first equation, $f_0(t)$ is a constant (which we take to be 1).

To solve the second equation, we note that $[H(t) - E(t)]$ is invertible on the subspace orthogonal to $\Phi(t)$. Applying this restricted resolvent operator $[H(t) - E(t)]_r^{-1}$, we obtain

$$\psi_1(t) \;=\; f_1(t)\,\Phi(t) \;+\; \psi_1^{\perp}(t),$$

where $\psi_1^{\perp}(t) \;=\; i\,[H(t) - E(t)]_r^{-1}\,\dot{\Phi}(t)$, and $f_1(t)$ is not yet determined.

Completing the Proof of Theorem 1

Arbitrarily choose $f_1(t) = 0$. The lemma then shows that

$$\psi_\epsilon(t) \;=\; e^{-i\int_0^t E(s)\,ds/\epsilon}\,\left(\,\psi_0 \;+\; \epsilon\,\psi_1^{\perp}\,\right)$$

agrees with an exact solution up to an $O(\epsilon)$ error.

The theorem follows since

$$e^{-i\int_0^t E(s)\,ds/\epsilon}\,\left(\,\psi_0 \;+\; \epsilon\,\psi_1^{\perp}\,\right) \;=\; e^{-i\int_0^t E(s)\,ds/\epsilon}\;\Phi(t) \;+\; O(\epsilon),$$

uniformly for $-T \le t \le T$.

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uniformly for $-T \le t \le T$.

Order $n \geq 2$. Write

$$\psi_j(t) \;=\; f_j(t)\,\Phi(t) \;+\; \psi_j^{\perp}(t).$$

Assume inductively that we have determined f_j for $j \leq n-2$ and $\psi_j^{\perp}$ for $j \leq n-1$.

Terms of order n require

$$i\,\frac{\partial \psi_{n-1}}{\partial t} \;=\; [H(t) - E(t)]\;\psi_n(t).$$

This implies

$$i\,\frac{\partial f_{n-1}}{\partial t}(t)\,\Phi(t) \;+\; i\,f_{n-1}(t)\,\frac{\partial \Phi}{\partial t}(t) \;+\; i\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t)$$
$$= \;[H(t) - E(t)]\;\psi_n(t).$$

Once again, we split this into two conditions:

$$i\,\frac{\partial f_{n-1}}{\partial t}(t) \;+\; i\,\langle\,\Phi(t),\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t)\,\rangle \;=\; 0.$$

$$i\,f_{n-1}(t)\,\frac{\partial \Phi}{\partial t}(t) \;+\; i\,P_{\perp}(t)\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t) \;=\; [H(t) - E(t)]\;\psi_n(t),$$

where $P_{\perp}(t) \;=\; I \;-\; |\Phi(t)\rangle\,\langle\Phi(t)|$.

We obtain

$$f_{n-1}(t) \;=\; -\int_0^t \langle\,\Phi(s),\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(s)\,\rangle\;ds.$$

$$\psi_n^{\perp}(t) \;=\; i\,[H(t) - E(t)]_r^{-1}\left(f_{n-1}(t)\,\Phi'(t) \;+\; P_{\perp}(t)\,\frac{\partial \psi_{n-1}^{\perp}}{\partial t}(t)\right).$$

Theorem 2 now follows when we apply the lemma to

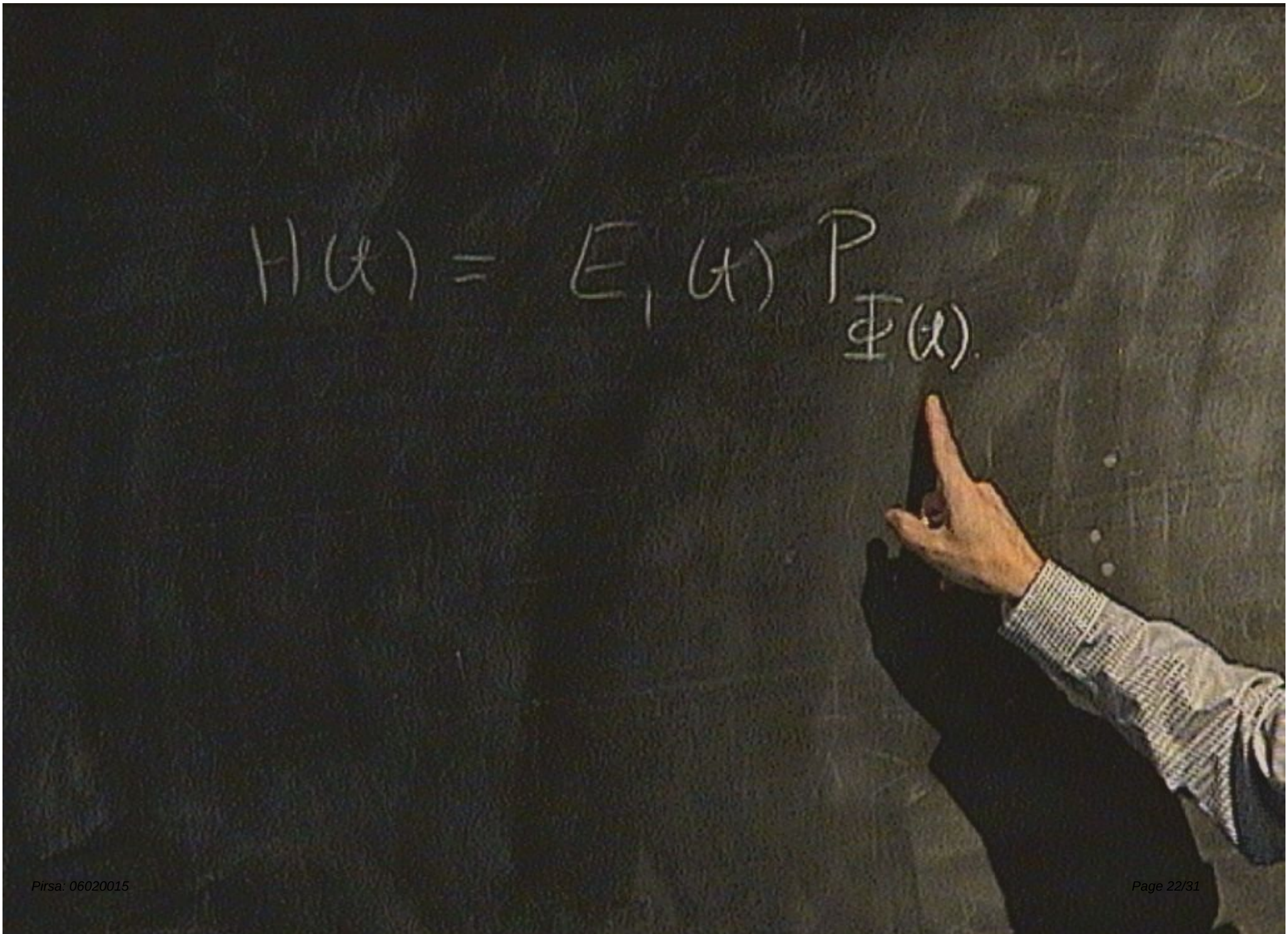
$$e^{-i\int_0^t E(s)\,ds/\epsilon}\left[\,\Phi(t) + \epsilon\,\psi_1(t) + \epsilon^2\,\psi_2(t) + \cdots + \epsilon^N\,\psi_N(t) + \psi^{\perp}_{N+1}(t)\,\right].$$

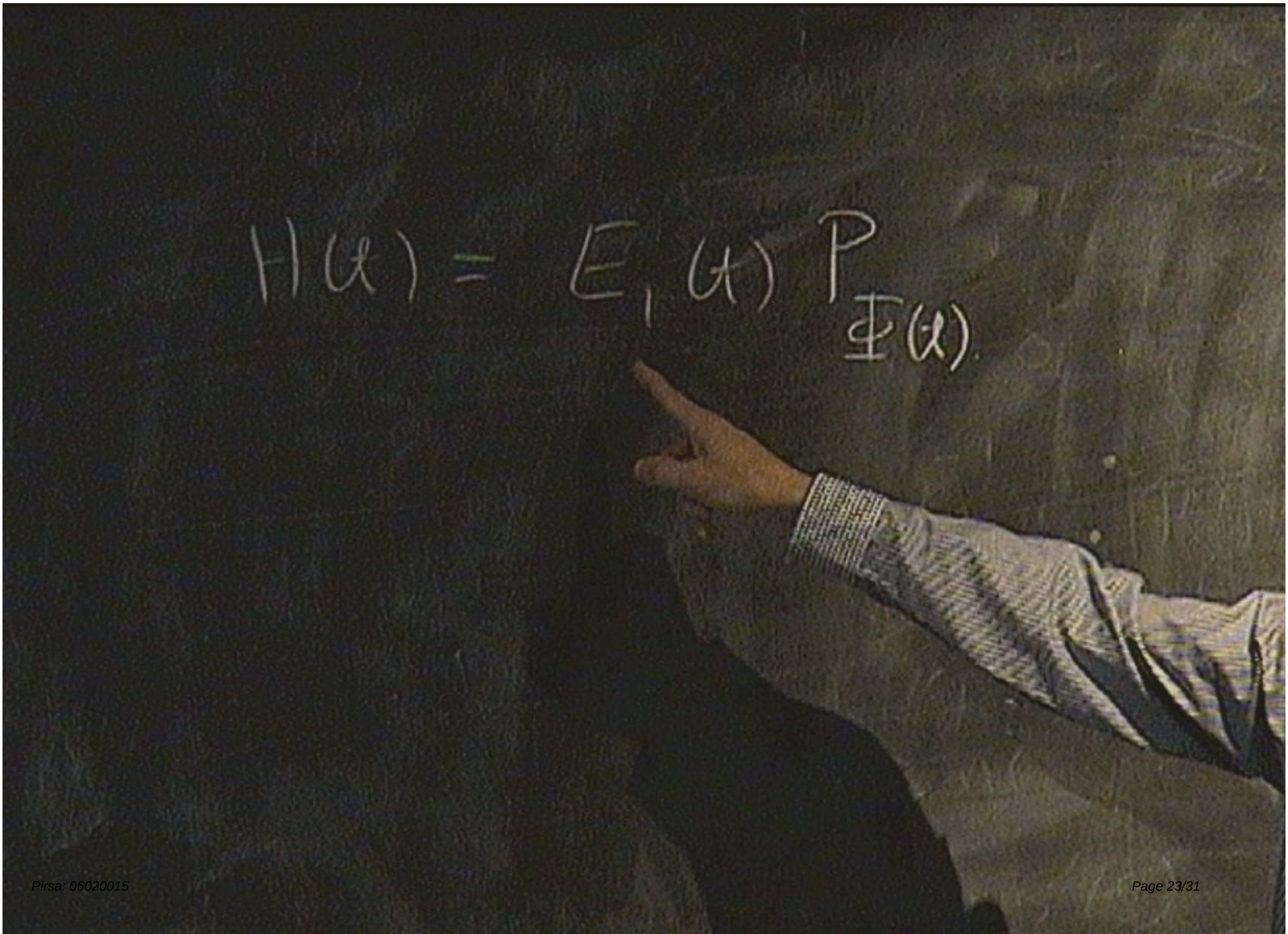
Comment about the error From this proof with $N \geq 2$, we see that the solution is a scalar times $\Phi(t)$ plus a phase times $\epsilon\,[H(t) - E(t)]_r^{-1}\,\dot{\Phi}(t)$ plus a term of order ϵ^2.

So, the exact solution is a scalar times $\Phi(t)$ plus an error whose precise leading order behavior is

$$\epsilon\,\|\,\dot{\Phi}(t)\,\|/g(t).$$

$$H(\mathcal{U}) = E_1(\mathcal{U})\, P_{\Phi(\mathcal{U})}$$


$H(u) = E_1(u)\, P_{\Phi(u)}$


$H(u) = E_1(u)\, P_{\Phi(u)}$

Improvements from the past 30 years or so

1. As mentioned earlier, under analyticity hypotheses, optimal truncation yields exponentially accurate approximations.

2. Suppose $H(t)$ is smooth and that $H(t) = H_-$ for $t < -T$ and $H(t) = H_+$ for $t > T$. Then one gets estimates that are uniform for all time. Furthermore, for $|t| > T$, the expansion becomes quite trivial. At every order, the $\psi_j^{\pm}(t)$ terms vanish for $|t| > T$. Generically, they do not vanish for $|t| < T$.

3. The same phenomenon occurs in scattering situations if $H(t)$ and its derivatives approach limits sufficiently rapidly as $t \to \pm\infty$. This generalizes to the exponential estimates if $H(t)$ is analytic in a strip around the real axis with appropriate uniformity assumptions.

4. By WKB techniques for complex t, one can obtain exponentially small transition amplitudes in scattering theory. In an appropriate sense, this justifies Landau's version of the Landau Zener formula. For generic avoided crossings, the gaps behave like $2\sqrt{a^2v^2T + c^2}$ for some a and c. The transition amplitude behaves like $\exp\left(-\frac{av^2}{2ac}\right)$

5. "Superadiabatic" approximations of Sir Michael Berry have recently been made rigorous in some circumstances. The underlying idea is first to do the optimal truncation (or something equivalent) to obtain a basis of very accurate approximate solutions. One then does a second perturbation expansion using that basis on the set of unperturbed states. In this way, in some cases, one can obtain the leading order exponentially small corrections. Under appropriate hypotheses, there is a universal time behavior for these corrections that roughly has the form of $C_1 e^{-C_2/\varepsilon^{1/2}} \sin(C_3/\varepsilon^{1/2} - \delta_0)/\varepsilon^{C_4}$

Improvements from the past 20 years or so.

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6. One can also generalize in other ways. For example, there are various results concerning Hamiltonians that do not have gaps.

7. One can allow the gap to go to zero at a finitely many points and still get estimates. Generically, the first correction to the main adiabatic term is $O(\epsilon^{1/2})$. Also, one generically obtains powers of ϵ times powers of $\log(\epsilon)$ at higher order.

A few other comments.

1. There is a non–generic, but slightly non–trivial explicitly sovable model.
Let $H(t)$ be the orthogonal projection onto the vector $\begin{pmatrix}\cos(t)\\ \sin(t)\end{pmatrix}$.

$$H(t) = \begin{pmatrix}\cos^2(t) & \cos(t)\sin(t)\\ \cos(t)\sin(t) & \sin^2(t)\end{pmatrix}.$$

Write $\psi(t) = c_1(t)\begin{pmatrix}\cos(t)\\ \sin(t)\end{pmatrix} + c_2(t)\begin{pmatrix}-\sin(t)\\ \cos(t)\end{pmatrix}$, and rewrite the Schrödinger equation in terms of the vector $\begin{pmatrix}c_1(t)\\ c_2(t)\end{pmatrix}$. This leads to a Schrödinger equation with time–independent Hamiltonian

$$\begin{pmatrix}1 & i\epsilon\\ -i\epsilon & 0\end{pmatrix},$$

which can clearly be solved explicitly.

2. By changing the time variable, one can move difficulties back and forth between the gap to the eigenvector for two–level systems. In particular, as long as there is a gap, one can replace t by $\int_0^t (E_1(s) - E_2(s))\,ds$ to obtain a new system whose the gap is constant. However, a small gap at some time for the original system translates into a large derivative for the eigenvector in the new system. (An example of the principle of Conservation of Difficulty.)

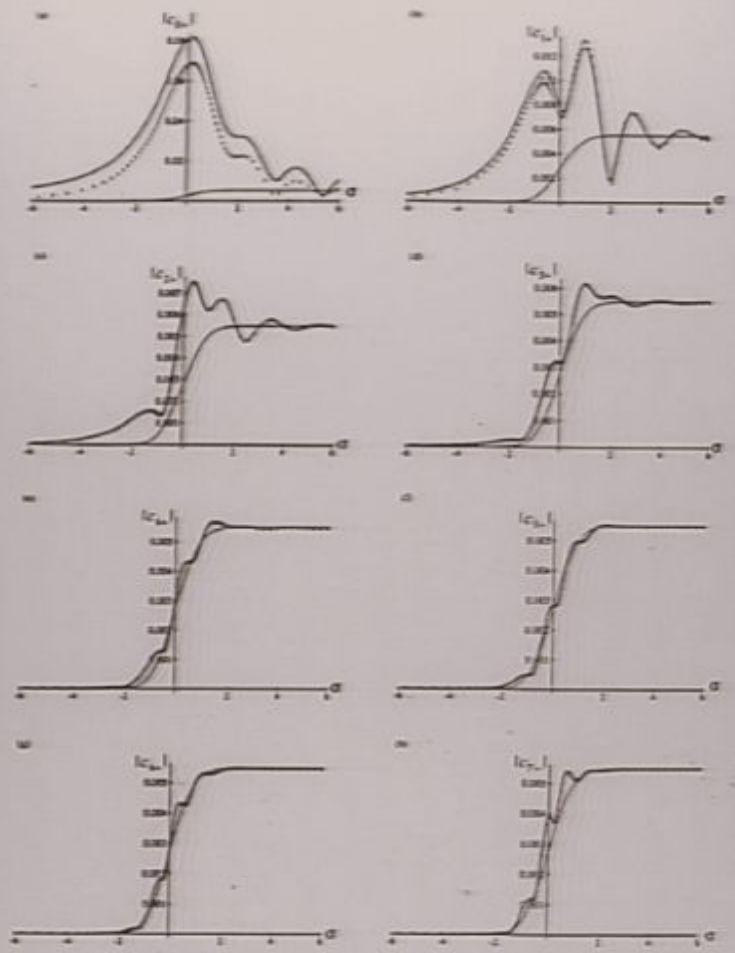

Figure 1. (*a*)–(*k*). Sequence of histories of transition amplitudes $|c_{+-}(\tau(\sigma))|$ in (*a*) the ordinary adiabatic basis $n=0$ and (*b*)–(*k*) the superadiabatic bases $n=1$–10, for the Landau–Zener Hamiltonian with $\varepsilon=0.2018$ (thick line) and the tanh Hamiltonian with $\varepsilon=0.25$ (dots). The thin line is the optimal superadiabatic error function (14), which as expected best fits the data for $n=5$ (figure 11(*f*)).

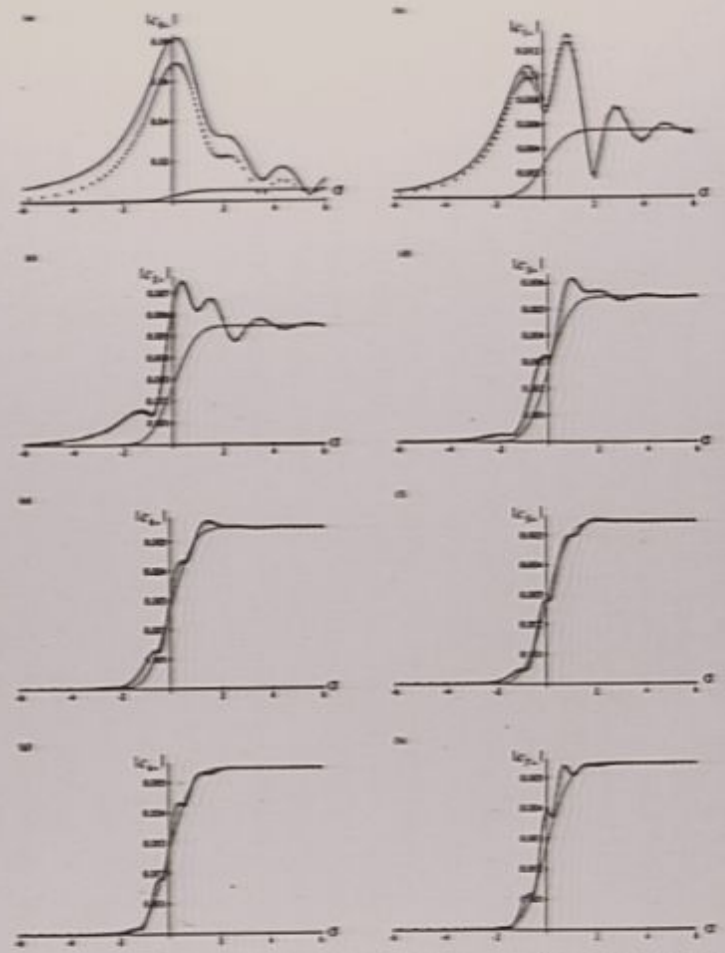

Figure 1. (a)–(k). Sequence of histories of transition amplitudes $|c_{n\to 1}(\sigma)|$ in (a) the ordinary adiabatic basis $n=0$ and (b)–(k) the superadiabatic bases $n=1$–10, for the Landau–Zener Hamiltonian with $\epsilon=0.3018$ (thick line) and the tanh Hamiltonian with $\epsilon=0.25$ (dots). The thin line is the optimal superadiabatic error function (14), which as expected best fits the data for $n=5$ (figure 1(*f*)).

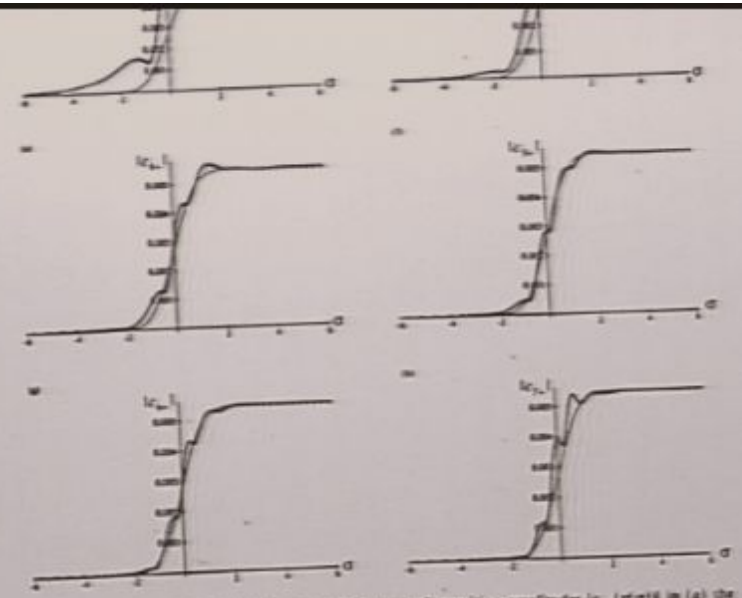

Figure 1. (a)–(k). Sequence of histories of transition amplitudes $|c_{n-1}(\tau(\sigma))|$ in (a) the ordinary adiabatic basis $n=0$ and (b)–(k) the superadiabatic bases $n=1$–10, for the Landau–Zener Hamiltonian with $\epsilon=0.3018$ (thick line) and the tanh Hamiltonian with $\epsilon=0.25$ (dots). The thin line is the optimal superadiabatic error function (14), which as expected best fits the data for $n=5$ (figure 1(*f*)).

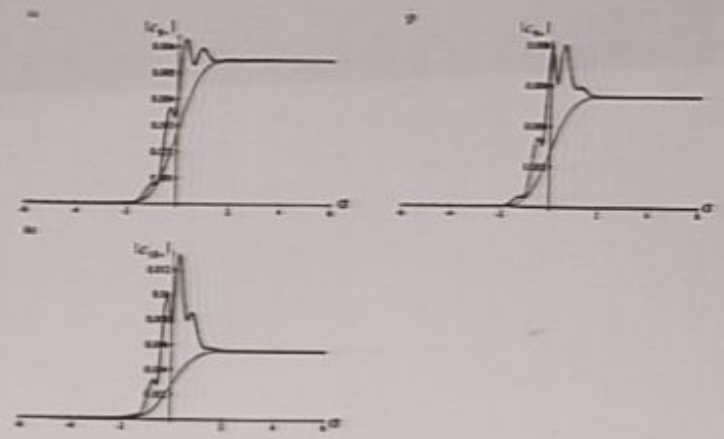

Figure 1. (continued).

The sequence of transition amplitude histories for the two models is shown in figure 1, for the superadiabatic bases $n=0$ through $n=10$. Instead of τ, we employ the natural variable σ defined in (14), that is we plot $|c_{n-1}(\tau(\sigma))|$. In the first few bases the two models give markedly different histories: the oscillations differ in amplitude (although they are similar in phase). The gradual attainment of universality as n approaches 5 is obvious. Not only do the two sets of histories become almost identical, but the

$$H(\alpha) = E_1(\alpha)\, P_{\Phi(\alpha)}$$

$$\begin{pmatrix} \alpha & 1 \\ 1 & -\alpha \end{pmatrix}$$

$$H(t) = E_1(t)\, P_{\Phi(t)}$$

$$\begin{pmatrix} 1 & \delta \\ \delta & -1 \end{pmatrix} \qquad \begin{pmatrix} \tanh t & \delta \\ \delta & -\tanh t \end{pmatrix}$$