Super-adiabatic transitions (Davydov sec. 92; Shapere and Wilczek p. 177)

- Suppose that the Hamiltonian $H(t)$ depends on time t but does so slowly. How slowly? So that the characteristic energy scale associated with the variation is much smaller than the separation between instantaneous energy eigenvalues.

- Also suppose that at each instant t the spectrum of $H(t)$ is discrete and nondegenerate:

quantum numbers

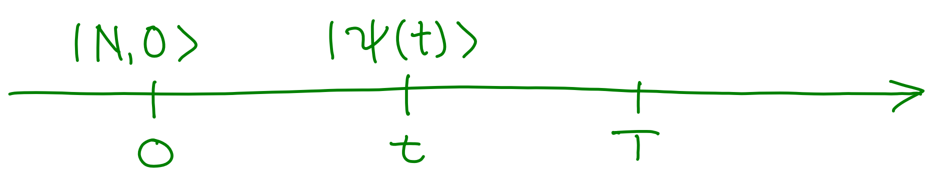
$$H(t)\,|n,t\rangle = \mathcal{E}_n(t)\,|n,t\rangle$$

instantaneous Hamiltonian — instantaneous eigenstates — instantaneous eigenvalues

(not Heisenberg-Schrödinger dynamics)

- Now consider the time evolution of an arbitrary Schrödinger-picture state $|\psi(t)\rangle$: $i\hbar \frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$

Choose as initial condition some instantaneous eigenket $|N,0\rangle$



- If the system is in the adiabatic limit (extremely slow variation of H with time) then, according to the adiabatic theorem, the system remains in the instantaneous eigenstate that it began in (ie its quantum numbers don't change although the actual quantum state does: $|N,0\rangle$ evolves into $\propto |N,t\rangle$).

- We are concerned with the breaching of the adiabatic theorem owing to the non-infinitesimal rate at which $H(t)$ varies.
  We anticipate very small amplitudes for the state to be in other instantaneous eigenstates. A.M. Dykhne's method [JETP 14 (1962) 941] gives us a general method for estimating the corresponding small probabilities, which has the virtue of being very easy to use.

- We work relative to the basis of (orthogonal, normalised) instantaneous eigenstates by writing

$$|\psi(t)\rangle = \sum_m a_m(t)\, |m,t\rangle \, \exp\left\{ \frac{-i}{\hbar} \int_0^t d\tau \, \mathcal{E}_m(\tau) \right\}$$

general state

unknown amplitudes

instantaneous eigenkets of $H(t)$

convenient to extract these phase factors

- Inserting into the Time Dependent Schrödinger equation gives

$$\sum_m \left(\dot{a}_m |m,t\rangle + a_m(t) \frac{d}{dt}|m,t\rangle \right) \exp\left\{ \frac{-i}{\hbar} \int_0^t d\tau\, \mathcal{E}_m(\tau) \right\} = 0$$

— the term arising from $\frac{d}{dt}$(phase factor) cancels with the one from $H(t)$ acting on the instantaneous eigenstates

- Taking the inner product with $|n,t\rangle$, for which $\langle n,t|m,t\rangle = \delta_{nm}$ gives

same time

omit $m=n$ as $\frac{d}{dt}\langle n,t|n,t\rangle = 0$

$$\dot{a}_n = -\sum_{m(\neq n)} a_m(t) \langle n,t| \frac{d}{dt}|m,t\rangle \exp \frac{-i}{\hbar}\int_0^t d\tau [\mathcal{E}_m(\tau) - \mathcal{E}_n(\tau)]$$

- Now integrate from the initial $(t=0)$ to the final $(t=T)$ time:

$$a_n(T) = a_n(0) - \int_0^T dt \sum_{m(\neq n)} a_m(t) \langle n,t| \frac{d}{dt}|m,t\rangle \times \exp \frac{-i}{\hbar}\int_0^t d\tau [\mathcal{E}_m(\tau) - \mathcal{E}_n(\tau)]$$

- And now iterate once and truncate to get

$$a_n(T) \approx \underbrace{a_n(0)}_{\delta_{n,N}} - \int_0^T dt \sum_{m(\neq n)} \underbrace{a_m(0)}_{\delta_{m,N}} \langle n,t| \frac{d}{dt}|m,t\rangle \times \exp \frac{-i}{\hbar}\int_0^t d\tau [\mathcal{E}_m(\tau) - \mathcal{E}_n(\tau)]$$

and examine $a_n(T)|_{n\neq N}$, as we are interested in <u>transition</u> amplitudes:

$$a_n(T)\Big|_{n\neq N} \approx -\int_0^T dt \langle n,t| \frac{d}{dt}|N,t\rangle \exp \frac{-i}{\hbar}\int_0^t d\tau [\mathcal{E}_N(\tau) - \mathcal{E}_n(\tau)]$$

- Next, we eliminate $\langle n,t|\frac{d}{dt}|N,t\rangle$ using the following result:

Take the time derivative of $H(t)|N,t\rangle = \mathcal{E}_N(t)|N,t\rangle$ to get

$$\frac{dH}{dt}|N,t\rangle + H(t)\frac{d}{dt}|N,t\rangle = \frac{d\mathcal{E}_N}{dt}|N,t\rangle + \mathcal{E}_N(t)\frac{d}{dt}|N,t\rangle$$

and apply $|n,t\rangle\big|_{n\neq N}$ to get

$$\mathcal{E}_n(t)\langle n,t|\frac{d}{dt}|N,t\rangle$$

$$\langle n,t|\frac{dH}{dt}|N,t\rangle + \langle n,t|H(t)|\frac{d}{dt}|N,t\rangle$$

$$= \frac{d\mathcal{E}_N}{dt}\underbrace{\langle n,t|N,t\rangle}_{0\ (\text{as } n\neq N)} + \mathcal{E}_N(t)\langle n,t|\frac{d}{dt}|N,t\rangle$$

and rearrange to get $\langle n,t|\frac{dH}{dt}|N,t\rangle = -\left(\mathcal{E}_n(t)-\mathcal{E}_N(t)\right)\langle n,t|\frac{d}{dt}|N,t\rangle$

Thus we arrive at

$$a_n(T)\big|_{n\neq N} \approx \int_0^T dt\ \frac{\langle n,t|\frac{dH}{dt}|N,t\rangle}{\mathcal{E}_n(t)-\mathcal{E}_N(t)}\exp\frac{-i}{\hbar}\int_0^t d\tau\left[\mathcal{E}_N(\tau)-\mathcal{E}_n(\tau)\right]$$

$$= \int_0^T dt\quad \Phi(t)\quad e^{-i\int_0^t d\tau\,\omega_{Nn}(\tau)}$$

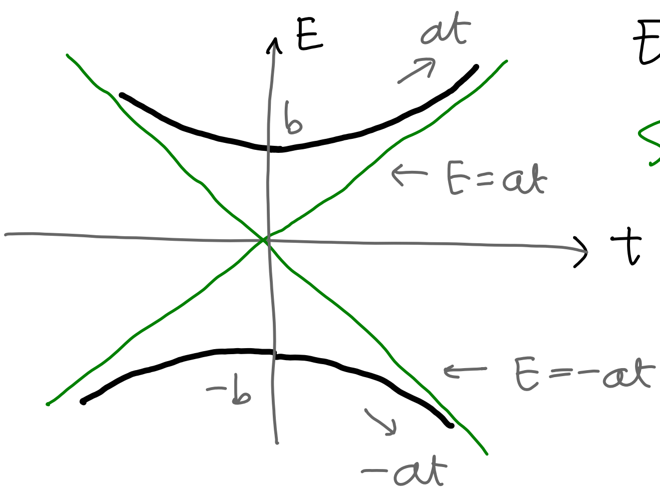
which we approximate using methods of complex variables.
(Note that denominator of $\Phi(t)$ and integrand of exponent are identical.)

- Consider $\Phi(t)$. As the instantaneous eigenvalue spectrum is nondegenerate it has no pole for t real; but there are poles at imaginary t (which we shall call z).

- For example, imagine that

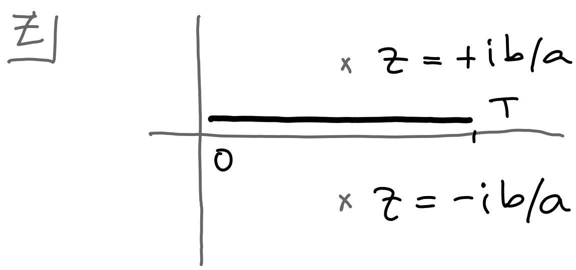
$$E_1 = -\sqrt{b^2+a^2t^2}$$
$$E_2 = +\sqrt{b^2+a^2t^2}$$

we shall see this instantaneous eigenvalue spectrum in the Landau-Zener problem



Then there is a pole at z such that $E_1(z) = E_2(z)$

ie $\sqrt{b^2+a^2z^2} = 0$, or $z = \pm ib/a$



poles of $\Phi(z)$ for this example

- Now back to generalities, and consider

$$a_n(T)\Big|_{n\neq N} = \int_0^T dt\, \Phi(t)\, e^{-i\int_0^t d\tau\, \omega_{Nn}(\tau)}$$

Our adiabaticity assumption makes ω_{Nn} large and allows us to use asymptotic methods.

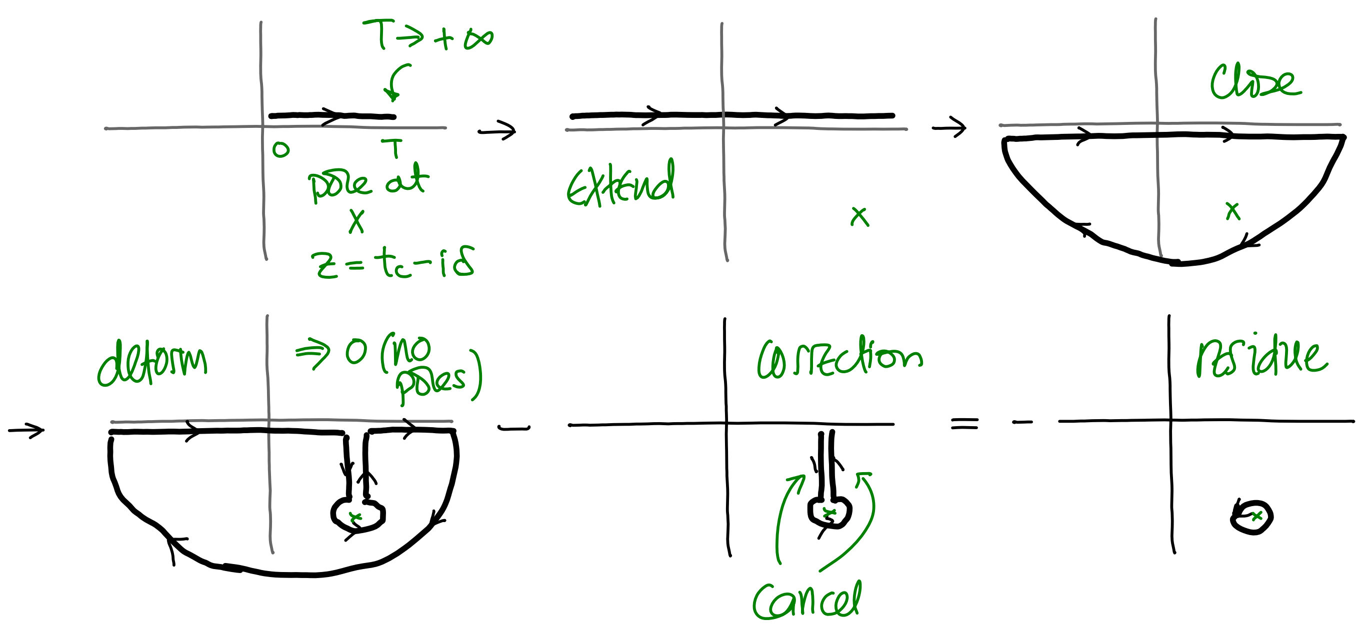
The pole nearest to the real z axis dominates (others give exponentially suppressed contributions, relatively).

We may extend the contour: $(0,T) \to (-\infty,+\infty)$.

And we may close it with a semicircle at infinity (which one depends on how ω_{Nn} behaves at $\pm i\infty$).

Note that the roots come in complex conjugate pairs (because the parameters in ω are real).

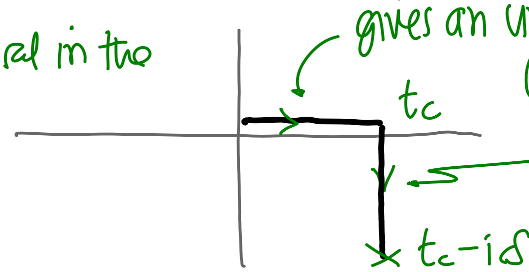
Suppose we close in the lower half plane:



The dominant (exponential) dependence comes from the phase factor

$$a_n(T)\Big|_{n\neq N} \sim \exp -i\int_0^{t_c - i\delta} dz\, \omega_{Nn}(z)$$

For the integral in the exponent



gives an unimportant phase factor (ω_{Nn} is real)

gives the important exponential dependence (ω_{Nn} becomes complex)

unimportant phase factor

real on (0 to t_c)

$$\exp\left\{-i\int_0^{t_c - i\delta} dz\, \omega_{Nn}(z)\right\} = \exp\left\{-i\int_0^{t_c} dz\, \omega_{Nn}(z)\right\}$$

Put: $z = t_c - iy$

$$\times \exp\left\{-i\int_{t_c}^{t_c - i\delta} dz\, \omega_{Nn}(z)\right\}$$

Im part gives... ...only a phase

$$\propto \exp -i\int_{y=0}^{y=\delta} (-i)\,dy\, \mathrm{Re}\,\omega_{Nn}(t_c - iy)$$

average on (t_c to $t_c - i\delta$)

$$= \exp\left\{-\delta\, \overline{\omega}_{Nn}\right\}$$

$$\overline{\omega}_{Nn} = \frac{1}{\delta}\int_{y=0}^{y=\delta} dy\, \mathrm{Re}\,\omega_{Nn}(t_c - iy)$$

[Choice of contour closing makes $\overline{\omega}$ positive]

depth of path

average on vertical path

So $$a_n(T\to\infty)\Big|_{n\neq N} \sim \exp -\delta\, \overline{\omega}_{Nn}$$

- Example application: Landau-Zener transition probability for upper (E_+) to lower (E_-) transition.

$$a_1 \sim \operatorname{Exp} - \int_{y=0}^{\delta} dy \; \mathrm{Re}\; \omega_{21}(t_c - iy)$$

$$\omega_{21}(z) = \frac{1}{\hbar}\left(E_2(z) - E_1(z)\right) = \frac{2}{\hbar}\sqrt{b^2 + a^2 z^2}$$

$\delta = b/a$ and $z = 0 - iy$

$$a_1 \sim \operatorname{Exp} - \int_0^{b/a} dy \, \frac{2}{\hbar}\sqrt{b^2 - a^2 y^2} \qquad \text{put } y = \frac{b}{a}\sin\theta$$

$$= \operatorname{Exp} - \frac{2b^2}{a\hbar}\int_0^{\pi/2} d\theta \, \cos^2\theta = \operatorname{Exp} - \frac{2b^2}{a\hbar}\,\frac{\pi}{2}\,\frac{1}{2}$$

Thus, the probability for the quantum-number-changing transition

$$P_{2\to 1} = |a_1|^2 \sim \operatorname{Exp}\left\{-\frac{b^2}{a}\frac{\pi}{\hbar}\right\}$$

$$= \operatorname{Exp} - 2\pi \cdot \left(b^2/2a\hbar\right)$$

↑

adiabaticity parameter
splitting (b) large and/or
H variation rate (a) small