Landau-Zener Transition

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We want to solve the Landau-Zener problem \[1\], which consists in solving the two-level problem when the frequency of the external field $\omega(t)$ varies across the resonant frequency $\omega_0$. This is known as a *chirped pulse*.

1 **Analytical Solution**

The two-level hamiltonian is

$$H = \hbar \begin{pmatrix} \omega_1 & \Omega^* \cos \omega t \\ \Omega \cos \omega t & \omega_2 \end{pmatrix} \tag{1}$$

Under the unitary transformation

$$\hat{U} \equiv \begin{pmatrix} e^{-i\omega_1 t} & 0 \\ 0 & e^{-i\omega_2 t} \end{pmatrix} \tag{2}$$

and the rotating-wave approximation, the system becomes\[4\]

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_g \\ c_e \end{pmatrix} = \hbar \begin{pmatrix} 0 & \Omega^* e^{i\delta t} \\ \Omega e^{-i\delta t} & 0 \end{pmatrix} \begin{pmatrix} c_g \\ c_e \end{pmatrix} \tag{3}$$

where the parameter $\delta(t) \equiv \omega(t) - \omega_0$ is defined as the detuning from the resonant frequency.

We are interested in the situation where the system is initially in the ground state

$$|c_g(t_i)|^2 = 1; \quad |c_e(t_i)|^2 = 0 \tag{4}$$

\[4\]The hamiltonian transforms as $H' = \hat{U}^\dagger (\hat{H} - i\hbar \partial_t) \hat{U}$
THERE IS AN ERROR IN THE FOLLOWING EQUATION (I HAVE ERRONEOUSLY ASSUMED A CONSTANT DELTA IN THE DERIVATION). THE CORRECT RESULT HAS A SIMILAR FORM THOUGH

Solving the eq.(3) for $c_e$ leads

$$\frac{d^2 c_e}{dt^2} + i\delta(t) \frac{d c_e}{dt} + \frac{\Omega^2}{4} c_e = 0 \quad (5)$$

with the initial conditions

$$c_e(t_i) = 0; \quad \frac{d c_e}{dt}(t_i) = -\frac{i\Omega}{2} e^{i\delta t_i} c_g(t_i) = \frac{\Omega}{2} \quad (6)$$

The eq.(5) can be easily solved numerically. However, there is an analytical solution when the frequency varies linearly in time. Let us consider $\delta(t) \equiv \alpha t$, and the change of variable $\tilde{c}_e \equiv e^{\frac{i\delta t}{4}} c_e$. The equation becomes

$$\frac{d^2 \tilde{c}_e}{dt^2} + \left( \frac{\Omega^2}{4} - \frac{i\alpha}{2} + \frac{\alpha^2 t^2}{4} \right) \tilde{c}_e = 0 \quad (7)$$

This equation can be written in a standard form via the change of variables $z \equiv \sqrt{\alpha} e^{-i\pi/4} t$ and $\nu \equiv \frac{i\Omega^2}{4\alpha} \quad [1]

$$\frac{d^2 \tilde{c}_e}{dz^2} + \left( \nu + \frac{1}{2} - \frac{z^2}{4} \right) \tilde{c}_e = 0 \quad (8)$$

This is the Weber differential equation \[2,3\], which has two independent solutions, $\tilde{c}_e = D_{-\nu-1}(-iz)$ and $\tilde{c}_e = D_{\nu}(z)$, where $D_{\nu}(z)$ is the parabolic cylinder function.

We conclude that the solution to eq.(5) is

$$c_e(t) = (a D_{-\nu-1}(-i\sqrt{\alpha} e^{-i\pi/4} t) + b D_{\nu}(\sqrt{\alpha} e^{-i\pi/4} t)) e^{-i\delta t/4} \quad (9)$$

where $a$ and $b$ are constants determined by the initial conditions.

When $t_i = -\infty$, there is an explicit solution for the asymptotic value of the excitation probability

$$|c_e(t \to \infty)|^2 \to 1 - e^{-\frac{\pi|\Omega|^2}{4\alpha}} \quad (10)$$

This result is called the Landau-Zener formula \[1\] (Recall that $\Omega$ is an angular frequency, and $\alpha$ is a rate of change in angular frequency)
2 Other forms

Experimentally, it is more convenient to work with linear frequencies. Let us define \( \Delta f \equiv f(t) - f_0 \equiv \delta/2\pi \) and \( f_R \equiv \Omega/2\pi \), then the eq.\((5)\) becomes

\[
\frac{d^2c_e}{dt^2} + 2\pi (f(t) - f_0) \frac{dc_e}{dt} + \pi^2 f_R^2 c_e = 0
\]

\[
c_e(t_i) = 0; \quad \frac{dc_e}{df}(t_i) = \pi f_R
\]  

(11)  

(12)

Also, we could use frequency as the independent variable instead of time. Let us assume a linear dependency in time \( f \equiv rt + f_i \), where \( r \) is the linear frequency rate of change. Then

\[
\frac{d^2c_e}{df^2} + 2\pi i \frac{f}{r} \frac{dc_e}{df} + \left( \frac{\pi f_R}{r} \right)^2 c_e = 0
\]

\[
c_e(f_i) = 0; \quad \frac{dc_e}{df}(f_i) = \frac{\pi f_R}{r}
\]

(13)  

(14)

and the Landau-Zener formula becomes

\[
|c_e(f \to \infty)|^2 \to 1 - e^{-\frac{\pi^2 f_R^2}{2r}}
\]

(15)

3 Numerical Calculation

![Figure 1: Excitation probability versus detuning for different sweep rates: \( r = 3f_R^2 \) (blue), \( r = 9f_R^2 \) (red). The initial detuning is \( \Delta f_i = -5f_R \). The dashed line is the Landau-Zener limit (\( \Delta f_i = -\infty \))](image-url)
Figure 2: Asymptotic value of the excitation probability for different initial detunings: $\Delta f_i = -f_R$ (blue), $\Delta f_i = -2f_R$ (red) and the Landau-Zener limit $\Delta f_i = -\infty$ (dashed)

4 Chirped pulse vs fixed frequency pulse

See ‘20131016 Raman sweep vs pulse.nb’

5 Conclusions

- Most of the excitation occurs in the frequency range $\delta \in [-\Omega, \Omega]$
- The sweep speed controls the excitation probability. A rule of thumb would be ‘a sweep rate $\alpha$ smaller than $\Omega^2$ gives an excitation level higher than 70%’

6 Beyond Simple Models

Other works explore analytical [4, 8] and numerical [9, 10] solutions for different sweep functions. The reference [11, 12] explores Landau-Zener transitions in three-level systems.

References


