Chapter 28

Application of Eigenvalues and Eigenvectors

28.1 Landau-Zener Problem

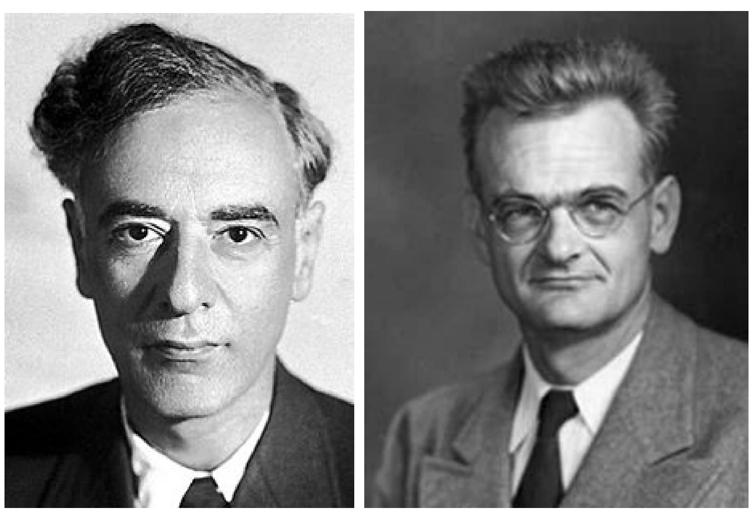

Figure 28.1: Lev Landau (left) and Clarence Zener (right). Landau solved this famous problem, but had an error in the coefficient of the exponent of his answer. Zener provided the correct derivation by mapping it to a complicated differential equation that had a special function solution (it is called the Weber equation and the solutions are parabolic cylinder functions).

We begin with a problem called the Landau-Zener problem. It is described by a 2×2 matrix

$$H = \begin{pmatrix} \delta t & v \\ v & -\delta t \end{pmatrix}. \tag{28.1}$$

Here, δ and v are real numbers and t is time. This matrix corresponds to the Hamiltonian of a two-state quantum-mechanical system whose uncoupled states are initially far away in energy, have their energy difference reduced linearly in time (with a rate given by δ) until it is zero at $t = 0$ and then it increases again to infinity as $t \to \infty$; but the energy level that is the lowest energy state switches. The v parameter describes how the two states are coupled together, which you should interpret as how easily can the system make a change from one state to another. If v is large, it does so easily. If v is small, it does so with difficulty. Don't worry if you don't understand why anything said above is correct or not, or what it means, if this seems too abstract to you. Just take what we do next as a purely mathematical exercise and know that it is meaningful for time-dependent quantum mechanics.

Th eigenvalues of this 2×2 matrix are found from solving

$$\det \begin{pmatrix} \delta t - E & v \\ v & -\delta t - E \end{pmatrix} = E^2 - (\delta t)^2 - v^2 = 0, \tag{28.2}$$

which is easily solved by

$$E = \pm\sqrt{(\delta t)^2 + v^2} \tag{28.3}$$

The plot, in Fig. 28.2, shows that the minimum energy gap is at $t = 0$ and the gap is equal to $2v$.

Note that as $t \to -\infty$, the lowest energy state has $E \to \delta t$ (recall, we have $t < 0$ here) and its eigenvector, called $\vec{e}_+$ is $\binom{1}{0}$. As $t \to +\infty$, the lowest-energy state has $E \to -\delta t$ and the eigenvector is $\vec{e}_-$ is $\binom{0}{1}$. So, as t runs from $-\infty$ to $+\infty$, *if the system stays in the lowest-energy state*, then the eigenstate will evolve from the initial one at $\vec{e}_+$ for $t = -\infty$ to the final one $\vec{e}_-$ for $t = +\infty$.

28.2 Quantum tunneling

In quantum mechanics, there can be tunneling, and the system can tunnel to the other state with some probability when $v \neq 0$. The Landau-Zener problem is to determine how to calculate this probability.

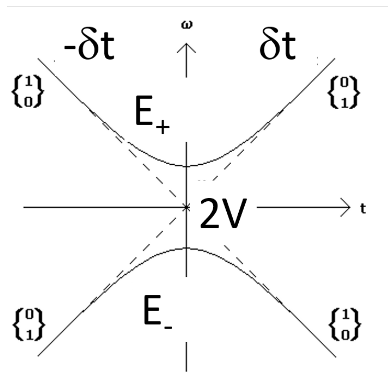

Figure 28.2: Schematic of the Landau-Zener transition. The solid lines, which are the two eigenvalues we calculated in Eq. (28.3), are the two instantaneous energy levels. They vary in time as shown above with what is called an avoided crossing at $t = 0$.

I won't be able to derive the full theory for how to solve this but will motivate the procedure for you. The parameter t is the time. Denote $\Psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$ as the wave function at time t. We start with $\Psi(t \to -\infty) = \binom{1}{0}$. The time-dependent Schrodinger equation is

$$i\hbar \frac{d}{dt}\Psi(t) = H(t)\Psi(t). \tag{28.4}$$

To solve this approximately, we discretize the derivative to have

$$i\hbar \frac{\Psi(t + \Delta t) - \Psi(t)}{\Delta t} = H(t)\Psi(t). \tag{28.5}$$

Our goal is to reorganize this equation so we can determine $\Psi(t + \Delta t)$ from $\Psi(t)$. So, moving the $\Psi(t)$ terms to the right hand side, we have

$$\Psi(t + \Delta t) = \left(1 - \frac{i}{\hbar} H(t)\Delta t\right)\Psi(t) = e^{-\frac{i}{\hbar}H(t)\Delta t}\Psi(t), \tag{28.6}$$

where in the last line we used the Taylor series expansion for the exponential function and the fact that we choose the time step Δt to be small. We then repeat the process, replacing $\Psi(t)$ by $\Psi(t - \Delta t)$, continuing until we get to $\Psi(t_0)$ as the starting point. The result is

$$\Psi(t + \Delta t) = e^{-\frac{i}{\hbar}H(t)\Delta t} e^{-\frac{i}{\hbar}H(t-\Delta t)\Delta t} e^{-\frac{i}{\hbar}H(t-2\Delta t)\Delta t} \ldots e^{-\frac{i}{\hbar}H(t_0)\Delta t}\Psi(t_0), \tag{28.7}$$

which is called the Trotter formula.

The probability to stay in the same eigenstate is $|\vec{e}_-(t=\infty)\cdot\Psi(t=\infty)|^2$. This is a postulate of quantum mechanics that you have to accept. To solve this problem, we start at an early time, pick a Δt, and multiply each of the "Trotter" factors to get to large time, which we approximate as infinity. Then we take the dot product and square it.

Unfortunately, we do not know how to compute this result analytically from the Trotter formula. It is true that the exponential of a 2×2 matrix can be computed exactly (which is a problem you work out in the lecture problems for this lecture). Unfortunately, we cannot determine the product of a chain of these exponentials. But, we can use this formula to determine the answer *numerically*. You need to experiment a bit with what value of t_0 you would want to start with, how small we should make Δt and how many steps we should include in the Trotter formula. But you will find, if you do this, that you can obtain a fairly accurate answer to the problem. Indeed, the correct result is that the probability to stay in the same eigenstate is $1-\exp(-\pi v^2/\delta)$. When Landau solved it, he did not correctly determine the factor π in the exponent. Give it a try and see if you get the right result!

28.3 Oscillations

We consider the problem of three ions confined in a one-dimensional trap. An image of ions in a trap is given in Fig. 28.3. I am always amazed by this. When I was in high school, textbooks would tell us that we could never image an atom. But, similar to the Dr. Seuss tale *Horton Hears a Who*, we can coax atoms to "tell us they are there." This is called a cycling transition. We shine light on atoms and they radiate the light out in all directions, similar to what you might call a nano reflector. So the figure shows images of *individual atoms* trapped in space!

There is a theorem in electromagnetism called Earnshaw's theorem that says one cannot trap a charged particle in a static electric field. So traps are constructed from time-varying fields that push in the right direction at the right time. They can be modeled by what are called pseudopotentials, which describe the trap using an effective static potential. It is simple, just a parabolic confining potential in one dimension with the repulsive Coulomb potential. The parabolic potential pulls the ions together, the Coulomb repulsion pushes them apart, the compromise is a lattice called a Wigner lattice.

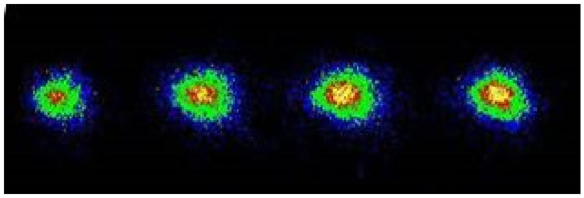

Figure 28.3: Image of light absorbed and then emitted from ions in a linear Paul trap undergoing a cycling transition. The balls of light come from individual ions in the trap.

We will work in dimensionless units where the potential is

$$V(x_1,x_2,x_3) = \frac{1}{2}k\left(x_1^2+x_2^2+x_3^2\right) + \frac{1}{|x_1-x_2|} + \frac{1}{|x_2-x_3|} + \frac{1}{|x_1-x_3|} \tag{28.8}$$

and the kinetic energy is

$$\frac{1}{2}\left(\frac{dx_1}{dt}\right)^2 + \frac{1}{2}\left(\frac{dx_2}{dt}\right)^2 + \frac{1}{2}\left(\frac{dx_3}{dt}\right)^2. \tag{28.9}$$

The dimensionless units allow us to set $e^2 = 1$ and $m = 1$. You are not expected to see why without making the change to the dimensionless variables yourself.

For equilibrium, we need $\frac{\partial V}{\partial x_i} = 0$ for each ion

$$\implies -kx_1 - \frac{1}{(x_1-x_2)^2} - \frac{1}{(x_1-x_3)^2} = 0 \tag{28.10}$$

$$\implies -kx_2 + \frac{1}{(x_1-x_2)^2} - \frac{1}{(x_2-x_3)^2} = 0 \tag{28.11}$$

$$\implies -kx_3 + \frac{1}{(x_1-x_3)^2} + \frac{1}{(x_2-x_3)^2} = 0. \tag{28.12}$$

The solution is $x_2^0 = 0$, $x_1^0 = -x_3^0 = -(\frac{5}{4k})^{\frac{1}{3}}$. Please work out this algebra yourself.

We examine oscillations about equilibrium $x_1 = x_1^0 + \delta x_1$, $x_2 = x_2^0 + \delta x_2$, $x_3 = x_3^0 + \delta x_3$. We substitute into the potential and expand through second order in δx_i^2 yielding

$$\begin{aligned}
V(x_1,x_2,x_3) = \quad & \tfrac{1}{2}k(x_1^0)^2 + kx_1^0\delta x_1 + \tfrac{1}{2}k(\delta x_1)^2 \\
& +\tfrac{1}{2}k(x_2^0)^2 + kx_2^0\delta x_2 + \tfrac{1}{2}k(\delta x_2)^2 \\
& +\tfrac{1}{2}k(x_3^0)^2 + kx_3^0\delta x_3 + \tfrac{1}{2}k(\delta x_3)^2 \\
& +\tfrac{1}{|x_1^0-x_2^0|} + \tfrac{-\delta x_1+\delta x_2}{(x_1^0-x_2^0)^2} + \tfrac{1}{2}\tfrac{\delta x_1^2-2\delta x_1\delta x_2+\delta x_2^2}{|x_1^0-x_2^0|^3} \\
& +\tfrac{1}{|x_2^0-x_3^0|} + \tfrac{-\delta x_2+\delta x_3}{(x_2^0-x_3^0)^2} + \tfrac{1}{2}\tfrac{\delta x_2^2-2\delta x_2\delta x_3+\delta x_3^2}{|x_2^0-x_3^0|^3} \\
& +\tfrac{1}{|x_1^0-x_3^0|} + \tfrac{-\delta x_1+\delta x_3}{(x_1^0-x_3^0)^2} + \tfrac{1}{2}\tfrac{\delta x_1^2-2\delta x_1\delta x_3+\delta x_3^2}{|x_1^0-x_3^0|^3},
\end{aligned} \tag{28.13}$$

where the first terms in each line are constants and the total of the second terms in each line vanishes due to the condition of equilibrium. The potential can then be rewritten in the "compact" way

$$\begin{aligned}
& V(x_1,x_2,x_3) = V(x_1^0,x_2^0,x_3^0) + \\
& \tfrac{1}{2}\left(\delta x_1 \; \delta x_2 \; \delta x_3\right) \cdot \begin{pmatrix} \frac{1}{\left|x_1^0-x_2^0\right|^3}+\frac{1}{\left|x_1^0-x_3^0\right|^3}+k & -\frac{1}{\left|x_1^0-x_2^0\right|^3} & -\frac{1}{\left|x_1^0-x_3^0\right|^3} \\ -\frac{1}{\left|x_1^0-x_2^0\right|^3} & \frac{1}{\left|x_1^0-x_2^0\right|^3}+\frac{1}{\left|x_2^0-x_3^0\right|^3}+k & -\frac{1}{\left|x_2^0-x_3^0\right|^3} \\ -\frac{1}{\left|x_1^0-x_3^0\right|^3} & -\frac{1}{\left|x_2^0-x_3^0\right|^3} & \frac{1}{\left|x_1^0-x_3^0\right|^3}+\frac{1}{\left|x_2^0-x_3^0\right|^3}+k \end{pmatrix} \cdot \begin{pmatrix} \delta x_1 \\ \delta x_2 \\ \delta x_3 \end{pmatrix}
\end{aligned} \tag{28.14}$$

Using the notation $\delta\vec{x} = (\delta x_1, \delta x_2, \delta x_3)$, this is a vector "spring" problem with an equation of motion given by

$$m\frac{d^2\delta\vec{x}}{dt^2} = -\mathbb{K}\delta\vec{x}, \tag{28.15}$$

with the matrix $\mathbb{K}$ equal to the matrix in Eq. (28.14).

Our goal is to determine the normal modes of motion of the ions. These are the motions of the ions that are regular and repeating with the same period for each ion. Hence, we must have that the deviations from equilibrium satisfy $\delta x_j(t) = \delta x_j^0 e^{iwt}$, with δx^0 constants, for a normal mode. Substituting this form into the equation of motion yields

$$mw^2\delta\vec{x}^0 = \mathbb{K}\delta\vec{x}_0. \tag{28.16}$$

This is an eigenvalue problem (the eigenvalue is $m\omega^2$ since $\mathbb{K}$ is a matrix and $\delta\vec{x}_0$ is a vector) that we will solve on the homework.