May 3

An Atom Coupled to the Continuum – part 2

In the previous lecture, we diagonalized the Hamiltonian for a problem with an atomic state coupled to a free-particle continuum. We found the eigenstates of H and computed the scattering amplitude. I would now like to study this same system from another point of view, as a time-dependent quantum mechanics problem in which we study the evolution from fixed initial conditions.

In particular, I would like to study the following question: Prepare the system so that, at time $t = 0$, it is in the atomic state $|0\rangle$. Because this state couples to continuum states, the state $|0\rangle$ will, after some time, transition to a continuum electron state, and the electron will escape to infinity. The state $|0\rangle$ is thus unstable and subject to decay. Can we compute the decay rate?

To analyze this problem, we need to solve the time-dependent Schrödinger equation associated with the Hamiltonian written in the previous lecture. This is the set of two equations

$$i\frac{\partial}{\partial t}\psi(\vec{r},t) = -\frac{\nabla^2}{2m}\psi(\vec{r},t) + \lambda\chi(\vec{r})\,\alpha(t)$$

$$i\frac{\partial}{\partial t}\alpha(t) = E_0\,\alpha(t) + \lambda\int d^3r'\,\chi^*(\vec{r}\,')\,\psi(\vec{r}\,',t)$$

to be solved subject to the initial conditions

$$\psi(\vec{r},t=0) = 0 \qquad\qquad \alpha(t=0) = 1$$

To solve these equations, I will use a technique called the *Laplace transform.* Essentially, this is a Fourier transform in time subject to some additional restrictions appropriate to an initial-value problem. For a function $f(t)$, I will write the Fourier transform as

$$f(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,e^{-i\omega t}\,\tilde{f}(\omega) \qquad\qquad \tilde{f}(\omega) = \int_{-\infty}^{\infty}dt\,e^{i\omega t}\,f(t)$$

Please note that the signs in the exponent are opposite with respect to my convention for a Fourier transform in space. It is useful to make this change, because then the transform variable ω, a frequency, corresponds to the energy in quantum mechanics.

To construct $\tilde{f}(\omega)$ from $f(t)$, we need to have $f(t)$ well defined for all t. For the Laplace transform, we define

$$f(t) = \begin{cases} 0 & t < 0 \\ f(t) & t \geq 0 \end{cases}$$

This is set up for a situation where the system is at rest for all times $t < 0$, then it receives a kick at $t = 0$ and responds in a way that is determined by a differential equation. The postulate that there is no response for $t < 0$ is the statement of causality: the system must respond only *after* a force has been applied.

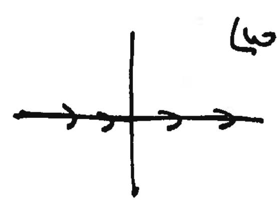
The expression for $\tilde{f}(\omega)$ can then be rewritten as

$$\tilde{f}(\omega) = \int_0^\infty dt \; e^{i\omega t} \, f(t)$$

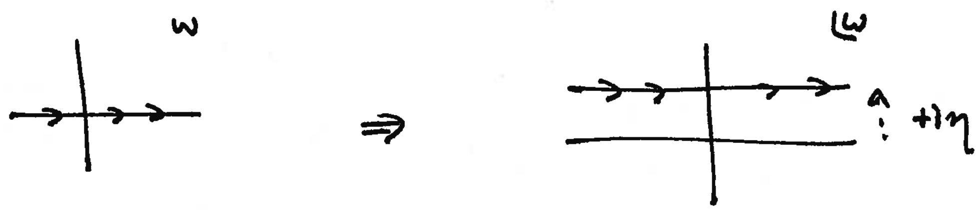
If the convergence of the integral is not obvious, we can define a convergent integral by adding a small positive imaginary part to ω, that is, by evaluating the integral at $\omega + i\epsilon$. Conversely, if the integral is well-defined for some ω, it will be even more well-defined if we add a positive imaginary part to ω. Then the function $\tilde{f}(\omega)$ will be nonsingular and, in fact, analytic for ω in the upper half of the complex plane.

The statement that $\tilde{f}(\omega)$ is analytic in the upper half ω plane gives us back causality by an interesting and important argument. Consider evaluating the integral

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \, e^{-i\omega t} \, \tilde{f}(\omega)$$



This complex contour integral is independent of the position of the contour, as long as the contour is not moved across any singularity of the integrand. Consider, then, moving the contour upward in the complex plane, $\omega \to \omega + i\eta$,



If $\tilde{f}(\omega)$ is analytic, we can make this move freely, since we do not encounter any singularity. The new value of the integral is

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, e^{\eta t}\, \tilde{f}(\omega + i\eta)$$

If $t < 0$, the value of the integral has decreased exponentially. If $\tilde{f}(\omega)$ does not grow exponentially as the contour is moved, we can push the contour to $+i\infty$ and find that

$$f(t) = 0 \quad \text{for } \underline{\text{all}} \quad t < 0$$

Here is an example of the use of the Laplace transform. Consider a damped harmonic oscillator

$$\frac{d^2}{dt^2} x + \gamma \frac{dx}{dt} + \Omega^2 x = 0$$

with the initial condition

$$x(t=0) = 0 \qquad \dot{x}(t=0) = A$$

That is, the oscillator starts at $x = 0$ and receives an initial kick at time zero. We would like to compute the subsequent motion of the oscillator. I will only consider the underdamped case in which γ is small.

To begin, compute the transform of the differential equation.

$$0 = \int_0^\infty dt \; e^{i\omega t} \left(\frac{d^2}{dt^2}x + \gamma \frac{d}{dt} x + \Omega^2 x \right)$$

We can move the derivatives off of the factors of $x(t)$ by integration by parts,

$$\int_0^\infty dt \; e^{i\omega t} \gamma \frac{d}{dt} x = \gamma e^{i\omega t} x \Big|_0^\infty - \int_0^\infty dt \; i\omega \, e^{i\omega t} \gamma x$$

$$\int_0^\infty dt \; e^{i\omega t} \frac{d^2 x}{dt^2} = e^{i\omega t} \dot{x} \Big|_0^\infty - i\omega \, e^{i\omega t} x \Big|_0^\infty + \int_0^\infty dt \, (i\omega)^2 e^{i\omega t} x$$

We imagine that ω has a small positive imaginary part, so $e^{i\omega t}$ vanishes as $t \to \infty$. Then the transform of the equation becomes

$$0 = -\dot{x}(0) + i\omega x(0) - \gamma x(0) - \omega^2 \hat{x}(\omega) - i\omega\gamma \hat{x}(\omega) + \Omega^2 \hat{x}(\omega)$$

$$0 = -A - (\omega^2 + i\omega\gamma - \Omega^2) \hat{x}(\omega)$$

and we can solve for $\tilde{X}(\omega)$

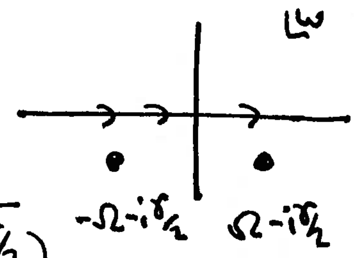
$$\tilde{x}(\omega) = - \frac{A}{\omega^2 + i\omega\gamma - \Omega^2}$$

Consider this as an analytic function of ω. Its singularities are poles at the zeros of the denominator

$$\omega_\pm = -i\gamma/2 \pm \left[\Omega^2 - \gamma^2/4\right]^{1/2} = -i\gamma/2 \pm \hat{\Omega}$$

There are two poles and, as required from the discussion above, both are in the lower half ω plane.

Now invert the transform

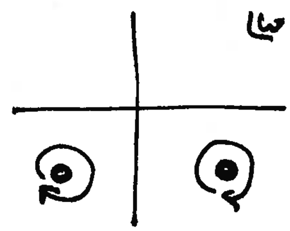


$$x(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \frac{-A}{(\omega - \hat{\Omega} + i\gamma/2)(\omega + \hat{\Omega} + i\gamma/2)}$$

Using the argument above, we already know that

$$x(t) = 0 \quad \text{for} \quad t < 0$$

For $t > 0$, the same argument says that we should evaluate the integral by pushing the contour *down* in the complex ω plane. We pick up the residues of the poles at $\omega = -i\gamma/2 \pm \hat{\Omega}$



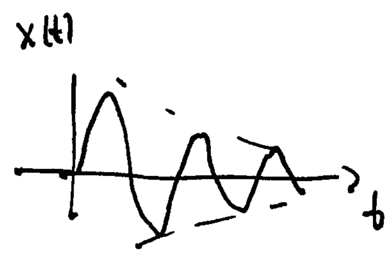
$$x(t) = (-2\pi i)\,\frac{1}{2\pi}(-A) \cdot \left[\frac{1}{2\hat{\Omega}} e^{-i\hat{\Omega}t} e^{-\gamma/2\, t} + \frac{1}{-2\hat{\Omega}} e^{i\hat{\Omega}t} e^{-\gamma/2\, t} \right]$$

The value of the integral is then

$$x(t) = \frac{A}{2i\hat{\Omega}} \left(e^{i\hat{\Omega}t} e^{-\gamma/2\, t} - e^{-i\hat{\Omega}t} e^{-\gamma/2\, t} \right)$$

or, finally,

$$x(t) = \frac{A}{\hat{\Omega}} \sin(\hat{\Omega}t)\, e^{-\gamma/2\, t}$$

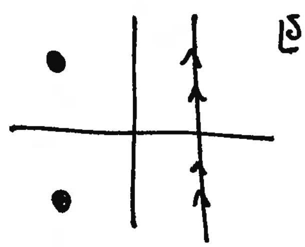


This behavior, an oscillation at a slightly shifted frequency, bounded by an exponential decay, is exactly what is expected.

In most treatments of the Laplace transform in textbooks, you will see a slightly different notation. The transform and its inverse are written

$$\tilde{f}(s) = \int_0^\infty ds\, e^{-st} f(t) \qquad\qquad f(t) = \int_{-\infty}^{\infty} \frac{ds}{2\pi i}\, e^{st}\, \tilde{f}(s)$$

The second integral is taken on a *vertical* contour in the complex s plane, to the *right* of all singularities of the integrand.



This is equivalent to the formalism above with the replacement $s = -i\omega$. In fluid dynamics, a fluid-mechanical instability corresponds to a pole moving from the left- to the right-hand side of the complex s plane. The causal contour is to the right of the singularities and is pushed to the left when evaluating for $t > 0$. A pole to the right of the y axis then gives an increasing exponential term in the solution.

We now return to the Wigner-Weisskopf problem. The time-dependent Schrödinger equation was given at the beginning of this lecture. We must now integrate it to form the Laplace transform. Integrating the ψ equation, we find

$$0 = \int_0^\infty dt\, e^{i\omega t} \left[i \frac{\partial}{\partial t}\psi + \frac{\nabla^2}{2m}\psi - \lambda \chi\, a(t) \right]$$

Integrate the first term by parts. This gives

$$0 = i\,\psi(\vec{r},t)\Big|_0^\infty - \int_0^\infty dt \left[(i\omega)\, e^{i\omega t}\, i\psi \right] + \int_0^\infty dt\, e^{i\omega t} \left[\frac{\nabla^2}{2m}\psi - \lambda \chi(\vec{r})\, a(t) \right]$$

Again, the boundary term vanishes at $t = \infty$. Also, our initial condition is $\psi(\vec{r}, t) = 0$ at $t = 0$. Then

$$0 = \omega \tilde{\psi}(\vec{r}, \omega) + \frac{\nabla^2}{2m} \tilde{\psi}(\vec{r}, \omega) - \lambda \chi(\vec{r}) \hat{\alpha}(\omega)$$

Similarly, the α equation is

$$0 = \int dt\, e^{i\omega t} \left[i \frac{\partial}{\partial t} \alpha - E_0 \alpha - \lambda \int d^3 r' \, \chi^*(\vec{r}') \psi(r', t) \right]$$

and, integrating by parts, this becomes

$$0 = -i + \omega \hat{\alpha}(\omega) - E_0 \tilde{\alpha}(\omega) - \lambda \int d^3 r \, \chi^*(\vec{r}') \tilde{\psi}(r', \omega)$$

It is useful to Fourier transform the ψ equation in space. This yields

$$0 = \left(\omega - \frac{p^2}{2m}\right) \tilde{\psi}(p, \omega) - \lambda \tilde{\chi}(p) \hat{\alpha}(\omega)$$

from which we can solve for $\tilde{\psi}(\vec{p}, \omega)$ in terms of $\tilde{\alpha}(\omega)$.

$$\tilde{\psi}(p, \omega) = - \frac{2m \lambda \hat{\chi}(p)}{p^2 - 2m\omega} \hat{\alpha}(\omega)$$

We can now insert this result into the α equation. The integral in the α equation can be evaluated using the trick discussed in the previous lecture.

$$\int d^3r' \, \chi^*(r') \Psi(r', \omega) = \int \frac{d^3q}{(2\pi)^3} \, \tilde{\chi}^*(q) \, \tilde{\Psi}(q, \omega)$$

Then

$$= \int \frac{d^3q}{(2\pi)^3} \, \tilde{\chi}^*(q) \left(-\frac{2m\lambda}{q^2 - 2m\omega} \right) \tilde{\chi}(q) \, \tilde{\alpha}(\omega)$$

We can recognize the integral over q as the integral $X(k)$ that we studied in the previous lecture

$$= -2m\lambda \cdot X\left(k = (2m\omega)^{1/2}\right) \cdot \tilde{\alpha}(\omega)$$

Putting the pieces together, we find

$$i = \left(\omega - E_0 + 2m\lambda^2 X\left((2m\omega)^{1/2}\right)\right) \tilde{\alpha}(\omega)$$

or

$$\tilde{\alpha}(\omega) = \frac{i}{\left(\omega - E_0 + 2m\lambda^2 X\right)}$$

We can recognize this structure from the previous lecture. There, we simplified this equation by writing

$$X(k) = \Sigma(k) + i \, H(k)$$

For weak coupling, the correction is important only in the region $\omega \approx E_0$, near the singularity. Then we can approximate Σ and H by their values at the singularity, and we find

$$\hat{\alpha}(\omega) = \frac{i}{\omega - E_* + i\,\Gamma/2}$$

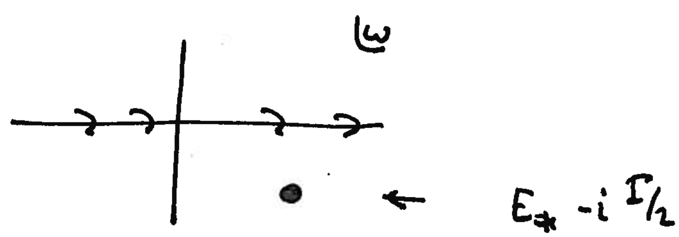
Now we can easily invert the Laplace transform. For $\alpha(t)$,

$$\alpha(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \frac{i}{\omega - E_* + i\,\Gamma/2}$$

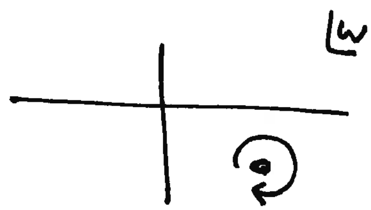
The integral is analytic in the upper half ω plane, as required. It has a pole at

$$\omega = E_* - i\,\Gamma/2$$

in the lower half plane.



If we evaluate the integral for $t < 0$, we push the contour upward and find that $\alpha(t) = 0$ for all $t < 0$. To evaluate the integral for $t > 0$, we push the contour downward



pick up the pole, and find

$$\alpha(t) = -2\pi i \frac{1}{2\pi} \quad i \cdot e^{-iE_* t} e^{-\Gamma/2\, t}$$

That is,

$$\alpha(t) = e^{-iE_* t} \; e^{-\frac{\Gamma}{2} t}$$

The probability that the system remains in the state $|0\rangle$ is then

$$|\alpha(t)|^2 = e^{-\Gamma t}$$

Thus, the probability that the system is in $|0\rangle$ decays exponentially

$$\text{Prob} = e^{-t/\tau} \qquad\qquad \tau = \frac{\hbar}{\Gamma}$$

The *half-life* is

$$t_{1/2} = \frac{\hbar \log 2}{\Gamma}$$

We have just derived the familiar – but still extremely weird – property of the decay of a quantum mechanical state. We cannot predict *when* the state will decay. We can only predict the *probability* of decay in a unit time interval, which is equal in every time interval. This leads to an exponential decay law for an ensemble of the unstable states.

The relation

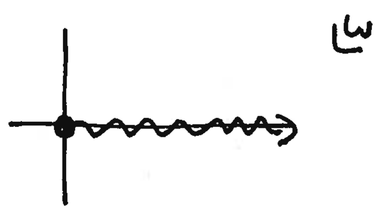
$$\tau = \frac{\hbar}{\Gamma}$$

is called the *Heisenberg uncertainty principle between energy and time.* The quantity Γ is the width of a resonance appearing in a scattering process. Essentially, the resonance is an extra state that blends into the free-particle continuum over a range of energies of width Γ. The quantity τ is the decay time of an unstable quantum state that couples to the continuum. We might think of the scattering process as the creation and decay of the unstable state. A large width means a short lifetime; a small width means a long lifetime. Typically, if a state is very long-lived, it is most useful to think of it as actually existing and decaying, while, if it is very short-lived, it is most useful to think of it as an ephemeral resonance in a scattering process. For intermediate values, these two situations go into one another smoothly.

There is a footnote that should be added to this discussion. I have not yet disclosed to you the full analytic structure of $\tilde{\alpha}(\omega)$ and $\tilde{\psi}(p,\omega)$. These quantities depend on

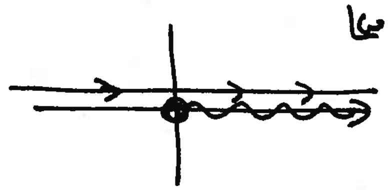
$$k = (2m\omega)^{1/2}$$

and therefore they will have a branch cut in the ω plane from 0 to ∞

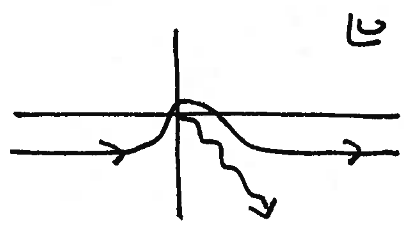


It can be shown that these quantities are analytic in the ω plane away from the branch cut. The contour of integration to invert the Laplace transform must be taken above all singularities, so, in particular, it must be taken to be above the cut. This is the clearest argument that the physical values of energy are to be taken just above the branch cut, at

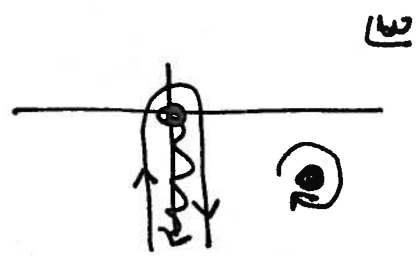
$$E = \frac{k^2}{2m} + i\epsilon$$



But, where is the resonance pole? To evaluate the transform for $t > 0$, we push the contour downward in the complex ω plane. A branch cut is not a fixed singularity, so we can analytically continue past the branch cut onto the next Riemann sheet or, equivalently, push the branch cut out of the way.



The resonance pole is located under the branch cut on the second Riemann sheet.



The contribution of the pole dies away as $e^{-\Gamma t/2}$. However, the part of the contour that sticks at $\omega = 0$ gives a contribution that dies away more slowly, as a power law $t^{-\alpha}$. This gives non-exponential corrections to the exponential decay law. In most systems of interest, these corrections, though formally dominant asymptotically, are extremely small.