# Simplified theory of level widths and exponential decay

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## 1. Introduction

Problems involving finite lifetimes and level widths arise in many different areas of quantum physics. For instance, in a world without weak interactions the neutron would be a stable particle, but in a more realistic treatment is actually decays to a proton, an electron, and an antineutrino. If we take another example from atomic physics, excited atomic states always sooner or later decays under emission of secondary particles to a ground state configuration plus some decay particles (electrons and/or photons). Typically, the decay is exponential in time, and if we analyze the energy distribution of decay particles we will find a Lorentzian of widths $\Gamma$ = Planck's constant / decay time. In problems of this kind, we are referring to some "zero-order" scheme where there is a discrete state *(e. g.* an excited atomic state), and a continuum involving the decay particles of interest, and there are continuum levels which are degenerate with the discrete state. In addition there is a perturbation which couples the discrete state and the continuum. To solve problems of this sort we may use a time space approach in which we study the evolution of a system originally prepared in the discrete state. Alternatively we may treat the problem in energy space and try to calculate how the discrete state may be decomposed into exact eigenstates of the full Hamiltonian including the perturbation. The two approaches are in fact equivalent.

Problems involving level widths can never be solved by finite-order perturbation theory. In time space, the probability that the system has not yet decayed involves an exponential, and such a function can not be formed from the perturbation $V$ to any finite order.

The rest of this tutorial is organized as follows. In Sec. 2 I describe a simple prototype lifetime problem and establish my notations. In Sec. 3 I show how first-order perturbation theory fails, and in the following section I show heuristically how the problems of first-order perturbation theory may be eliminated and how this leads to a broadening in energy space and to a decay in time space. The material up to this point is intended to fit into undergraduate courses in quantum mechanics based on, for example, the text by

Sakurai[1]. In Sec. 5 I show more rigorously how our prototype problem may be solved exactly, in the interest of those readers who would like to know more about the full story. In Sec. 6, finally, I give some brief historical notes.

## 2. A model lifetime problem

We imagine that we have an "unperturbed problem" with a sharp energy level "0" of energy $E_0$ and a continuum of levels "n" with energies $E_n$. A model of this kind may be used for describing, for instance, decay of excited atomic states under emission of photons. In such a case the sharp state "0" would be the initial excited atomic state without photons, and the continuum of states $|n>$ states where the atom is in its ground state and there is a photon $\mathbf{k}\omega$. Schematically we have

$$H = H_0 + V$$

$$H_0|0> = E_0|0> \tag{1}$$

$$H_0|n> = E_n|n>$$

and we will make the simplifying assumption the continuum states do not interact, *i. e.,* that

$$< n|V|m> = 0 \text{ when } n, m > 0\,, \tag{2}$$

and the diagonal element $<0|V|0>$ is considered to be absorbed in the definition of $H_0$. We will assume that the continuum of states "n" are degenerate with the sharp state "0". We imagine that the system under study is prepared in state "0" at an initial time ($t = 0$), and we want to obtain the state at later times.

We write the wave function in terms of unperturbed states

$$|\Psi(t)> = c_0(t)e^{-iE_0t}|0> + c_n(t)e^{-iE_nt}|n> \tag{3}$$

(we use units such that Planck's constant equals 1). From the time-dependent Schrödinger equation

$$i\,\frac{d}{dt}\,|\Psi(t)> = (H_0 + V)\,|\Psi(t)>$$

we obtain equations of motions for the amplitudes $c_n$:

$$i\,\dot{c_0}(t) = \sum_{n>0} <0|V|n>\, e^{i\omega_{0n}t}\, c_n(t), \tag{4a}$$

$$i\,\dot{c_n}(t) = < n|V|0>\, e^{i\omega_{n0}t}\, c_0(t) \tag{4b}$$

(see Sakurai, p. 327). Here $\omega_{nm} = E_n - E_m$ . So far no approximations have been made, and Eqs. (4) are thus completely equivalent to the exact time-dependent Schrödinger equation.

### 3. First-order perturbation theory

In first-order perturbation theory we work out $\Psi$ to linear order in $V$. This corresponds to inserting the zeroth-order approximation for $c_n$ in the RHS of Eqs. (4):

$$i\,\dot{c_0}(t) = 0,$$

$$i\,\dot{c_n}(t) = < n|V|0 > e^{i\omega_{n0}t}$$

which are readily solved to obtain

$$c_0 = 1, \tag{5a}$$

$$c_n(t) = -< n|V|0 > \frac{e^{i\omega_{n0}t} - 1}{\omega_{n0}} \tag{5b}$$

$$|c_n(t)|^2 = 2\pi\,| < n|V|0 > |^2\,\frac{2\sin^2\frac{1}{2}\,\omega_{n0}t}{\pi\,\omega_{n0}{}^2}\,. \tag{5c}$$

For times which are not too short but also not too long, Eq. (5c) reduces to the well-known "Golden Rule"

$$|c_n(t)|^2 \approx 2\pi\,t\,| < n|V|0 > |^2\,\delta(E_n - E_0) \tag{6}$$

(see Sakurai, pp. 328-335).

Unfortunately, first-order theory does not conserve the total probability, *i. e.,* the condition

$$|c_0(t)|^2 + \sum_{n>0} |c_n(t)|^2 = 1 \tag{7}$$

is violated. We notice that there is no correction to $c_0$ in first order (Eq. (5a)). However, an estimate how fast the initial state is depleted can be obtained from the first-order "Golden Rule":

$$|c_0(t)|^2 = 1 - \sum_{n>0} |c_n(t)|^2 \approx -\Gamma\,t \tag{8}$$

where

$$\Gamma = 2\pi \sum_{n>0} | < n|V|0 > |^2\,\delta(E_n - E_0) \tag{9}$$

First-order theory is valid as long as the depletion of the initial state "0" can be neglected, *i. e.,* as long as $\Gamma\,t \ll 1$.

**4. Treatment of decay and level widths**

We now attempt to remedy the first-order theory above from its most glaring defect, namely the violation of the norm condition in Eq. (7). For small times the depletion rate is given by Eq. (9). However, the change in $c_0$ is driven by the coefficients $c_n$ which in turn are driven by $c_0$ *(cf.* Eqs. (4)). Thus, is is reasonable to assume that the depletion rate is proportional to $|c_0(t)|^2$:

$$\frac{d}{dt}|c_0(t)|^2 = -\Gamma\,|c_0(t)|^2 , \tag{10}$$

which corresponds to an exponential decay

$$|c_0(t)|^2 = e^{-\Gamma t} . \tag{11}$$

In order to obtain the coefficients $c_n$ for continuum states we need the amplitude $c_0$ rather than the norm of the initial state. Clearly, Eq. (11) implies that

$$c_0(t) = e^{i\,h(t) - \frac{1}{2}\Gamma t} .$$

where $h(t)$ is some real function, and a more detailed analysis shows that $h(t)$ is a linear function of time. Thus,

$$c_0(t) = e^{-i(\Delta - \frac{1}{2} i\Gamma)t} . \tag{12}$$

We have now a possibility to obtain the distribution of final states for long times. We insert out result for the initial-state amplitude, Eq. (12), in the exact Eq. of motion, Eq. (4b). This gives

$$c_n(t) = -< n|V|0 > \frac{e^{i(E_n - E_0 - \Delta - \frac{1}{2} i\Gamma)t} - 1}{E_n - E_0 - \Delta + \frac{1}{2}\, i\Gamma} . \tag{13}$$

For long times the exponential in Eq. (13) tends to zero, and we find a Lorentzian probability distribution:

$$|c_n(\infty)|^2 = \frac{|< n|V|0 >|^2}{(E_n - E_0 - \Delta)^2 + \Gamma^2/4} \tag{14}$$

The exponential decay law corresponds to a measurement where we inspect the system after a given time and look if it has decayed or not. There is then no possibility to obtain the spectrum of decay particles, (spectrum of emitted photons, etc). The energy distribution in Eq. (14) corresponds to a complementary measurement when we observe the energy spectrum of decay particles that hit our spectrometer during a very long observation time. In this case it is not possible to say exactly *when* the decay actually took place.

Finally we want to verify that the total probability is conserved. After a long time all probability has been transferred to the continuum states "n".

Thus the total probability is

$$\sum_{n>0} |c_n(\infty)|^2 = \sum_{n>0} \frac{|<n|V|0>|^2}{(E_n - E_0 - \Delta)^2 + \Gamma^2/4} = \int \frac{d\varepsilon}{2\pi} \frac{\gamma(\varepsilon)}{(E_n - E_0 - \Delta)^2 + \Gamma^2/4} \quad (15)$$

where we have introduced

$$\gamma(\varepsilon) = 2\pi \sum_{n>0} |<n|V|0>|^2 \, \delta(E_n - \varepsilon) \,. \quad (16)$$

In Eq. (15) the region around $\varepsilon = E_0 + \Delta$ gives the dominating contribution, which allows us to approximate $\gamma(\varepsilon)$ with the value at the peak, $\gamma(E_0 + \delta)$. The integral is then easily calculated, and we we find a total probability

$$P_{tot} = \frac{\gamma(E_0 + \Delta)}{\Gamma}$$

Thus, the the parameter $\Gamma$ should be chosen such that this ratio is unity, which is very close to the first-order result in Eq. (9).

## 5. Justifications

In this section I will justify the basic results more rigorously. This material is really above what is required in an undergraduate presentation of quantum mechanics and it requires some knowledge of analytic functions and of Fourier integrals.

The model lifetime problem in Eqs. (1-2) can actually be solved exactly, and the the solution is most easily obtained in Fourier space. The equations of motions, Eqs. (4), are valid for positive times and are to be solved with the initial values $c_0 = 1$ , $c_n = 0$ for $t = 0$. We first make a formal trick and solve them for all times with initial values $c_0 = c_n = 0$ at $t = -\infty$. We account for the initial value at $t = 0$ by adding a source term $i\delta(t)$ to Eq. (4a):

$$i\,\dot{c_0}(t) = \sum_{n>0} <0|V|n> e^{i\omega_{0n}t}\, c_n(t) + i\,\delta(t) \,. \quad (4a')$$

For negative times, the equations (4a’, 4b) give amplitudes which are zero and they have no physical meaning. At time $t = 0$ the source term lifts $c_0$ to unity, and for $t > 0$ the solution agrees with that of the original problem. Because the amplitudes are now defined for all times we can perform a Fourier transformation:

$$c_n(t) = \int \frac{d\varepsilon}{2\pi}\, c_n(\varepsilon)\, e^{i(E_n - \varepsilon)t} \,. \quad (17)$$

In Fourier space, time derivatives are mapped to multiplications with $i(E_n - \varepsilon)$:

$$(\varepsilon - E_0) c_0(\varepsilon) = \sum_{n>0} <0|V|n> c_n(\varepsilon) + i, \quad (4a'')$$

$$(\varepsilon - E_n) c_n(\varepsilon) = <n|V|0> c_0(\varepsilon) \quad (4b'')$$

The correct solution of Eq. (4b") is

$$c_n(\varepsilon) = \frac{< n|V|0 >}{(\varepsilon - E_n + i\eta)}\, c_0(\varepsilon)\,, \tag{18}$$

where $\eta$ is a positive infinitesimal to ensure that $c_n(\varepsilon)$ is analytic in the upper half plane $\mathrm{Im}\,\varepsilon \geq 0$ including the real axis. The analyticity in Fourier space makes the time-space function $c_n(t)$ zero for negative times as it should. For negative times, we can close the integration contour in Eq. (17) by a large semicircle in the upper halfplane. The exponential function in Eq. (17) tends to zero in the upper half plane, and when the radius of the semicircle tends to infinity it will give no contribution to the integral. The integrand in analytic in the region bounded by the integration contour, and thus the entire integral is zero by virtue of Cauchy's theorem. Thus, if a Fourier transform is analytic in the upper halfplane, the corresponding time function is identically zero for negative times.

We have now eliminated $c_n$ and by inserting Eq. (18) in Eq. (4a") we obtain

$$(\varepsilon - E_0)c_0(\varepsilon) = \sum_{n>0} \frac{| < 0|V|n > |^2}{\varepsilon - E_n + i\eta}\, c_0(\varepsilon) + i$$

which can be simplified to

$$c_0(\varepsilon) = \frac{i}{\varepsilon - E_0 - \Sigma(\varepsilon)} \tag{19}$$

where

$$\Sigma(\varepsilon) = \sum_{n>0} \frac{| < 0|V|n > |^2}{\varepsilon - E_n + i\eta} = \int \frac{d\varepsilon'}{2\pi}\, \frac{\gamma(\varepsilon')}{\varepsilon - \varepsilon' + i\eta}\,, \tag{20}$$

is a "self energy" which renormalized the initial state. Eqs. (18-20) gives the exact solution to our problem. No approximations have been made, and thus there is no violation of the norm condition expressed in Eq. (7). Eq. (20) defines a function which is analytic in the upper half plane and whose imaginary part is strictly positive. Thus the denominator in Eq. (19) is never zero, and also $c_0(\varepsilon)$ is analytic as it should.

The self energy $\Sigma(\varepsilon)$ may be decomposed in real and imaginary parts as follows:

$$\mathrm{Re}\,\Sigma(\varepsilon) \equiv \Delta(\varepsilon) = P\int \frac{d\varepsilon'}{2\pi}\, \frac{\gamma(\varepsilon')}{\varepsilon - \varepsilon'}\,,\ \ \mathrm{Im}\,\Sigma(\varepsilon) = -\tfrac{1}{2}\,\gamma(\varepsilon)\,, \tag{21}$$

where we have made use of the identity

$$\frac{1}{x + i\eta} \rightarrow \frac{P}{x} - i\pi\,\delta(x) \text{ when } \eta \rightarrow \infty$$

(*cf.* Appendix A; $P$ stands for Cauchy's principal value). As will become clear in the following, the real part corresponds to a level shift, and the imaginary part to a lifetime width.

Finally we evaluate the amplitudes in time space. For short times, they will depend on the details of the state density function (Eq. (16)), but as we we show, they give an exponential decay law for times large compared with typical eigenfrequencies in $H_0$.

The solution for $c_0(\varepsilon)$ is a function which is strongly peaked around the value $\varepsilon_0 \equiv E_0 + \Delta_0$ where the real part of the dominator vanishes:

$$\varepsilon_0 - E_0 - \Delta(\varepsilon_0) = 0$$

If the decay is weak (small perturbation) we have approximately

$$\varepsilon_0 = E_0 + \Delta(E_0)\,,$$

and making a Taylor expansion of the denominator in Eq. (19) we find

$$\varepsilon - \Sigma(\varepsilon) \approx (1 - \frac{d\Delta(\varepsilon)}{d\varepsilon})\,(\varepsilon - \varepsilon_0 + \tfrac{1}{2}\,i\gamma(\varepsilon_0)) \equiv (\varepsilon - E_0 - \Delta_0 + \tfrac{1}{2}\,i\Gamma_0))\,/\,Z.$$

Thus,

$$c_0(\varepsilon) = i\,\frac{Z}{\varepsilon - E_0 - \Delta_0 + \tfrac{1}{2}\,i\Gamma_0} + \text{a smooth function of } \varepsilon.$$

which in time space corresponds to

$$c_0(t) = Ze^{-i(\Delta_0 - i\Gamma_0)t} \text{ plus smaller terms.}$$

The determination of final-state amplitudes $\{c_n\}$ then proceeds as in the previous section. The asymptotic time-space behavior shows that we can interpret $\Delta_0$ as a shift and $\Gamma_0$ as a damping of the discrete state.

The amplitude $c_0(\varepsilon)$ actually gives the decomposition of the initial state "0" into exact eigenstates of $H_0 + V$. Let the exact eigenstates be $\Psi(\varepsilon)$ normalized as

$$< \Psi(\varepsilon) | \Psi(\varepsilon') > = 2\pi\,\delta(\varepsilon - \varepsilon')\,.$$

The time-space coefficient $c_0(t)$ is just the overlap between the discrete state "0" and the exact wave function which starts out as $|0>$ at time zero:

$$|\Psi(t)> = \int \frac{d\varepsilon}{2\pi}\, e^{-i\varepsilon t} < \Psi(\varepsilon)|0> |\Psi(\varepsilon)>$$

*i. e.,*

$$< 0|\Psi(t)> = \int \frac{d\varepsilon}{2\pi}\, e^{-i\varepsilon t}\, | < 0|\Psi(\varepsilon)> |^2\,.$$

On the other hand we can write

$$< 0|\Psi(t) > = \int \frac{d\varepsilon}{2\pi} e^{-i\varepsilon t}(c_0(\varepsilon + i\eta) + c^{*_0}(\varepsilon - i\eta))$$

where $c_0{}^*(\varepsilon - i\eta)$), which is analytic in the lower half plane, gives the contribution for $t < 0$ and zero contribution for positive times. Thus,

$$2\,\mathrm{Re}\,c_0(\varepsilon) \equiv \frac{\gamma(\varepsilon)}{|\varepsilon - E_0 - \Sigma(\varepsilon)|^2} = |< 0|\Psi(\varepsilon) >|^2 ,$$

which incidentally is also the exact energy distribution of final states. Thus, the state "0" is a wave packet of exact eigenstates centered around the energy $E_0 + \Delta_0$ and with a spread $\Gamma_0$.

In conclusion, a more detailed analysis of our model lifetime problem essentially justifies the more heuristic arguments used in the previous section. We have also found a renormalization factor

$$Z = \frac{1}{1 - \dfrac{d\Delta}{d\varepsilon}}$$

which is close to unity for weak interactions, and more precise definitions of the level width

$$\Gamma_0 \approx \gamma(E_0 + \Delta_0) / Z$$

and of the level shift

$$\Delta_0 = \Delta(E_0 + \Delta_0)$$

## 6. Concluding remarks

The material in Section 3 was essentially developed by Wigner and Weisskopf[2] in the early days of quantum mechanics. The technique with coupled equation used in the more rigorous treatment I borrowed from Heitler[3], and it has close connections with what is usually referred to as "formal scattering theory", as introduced by Gell-Mann and Goldberger[4] in the fifties. An interesting alternative approach was introduced by Fano[5] in the sixties in a work on resonant excitation of doubly excited states in the helium atom. Fano view the problem as a time independent problem of finding the exact eigenstates of $H_0 + V$ and obtain an exact solution by direct diagonalization.

If we would apply the procedure outlined here to the case of radiative decay of atomic states, the shift $\Delta$ is a radiative correction to the atomic level under consideration, usually referred to as the "Lamb shift" after W. E. Lamb and R. C. Retherford who discovered the effect experimentally in 1947. (The model discussed here only accounts for the shift to leading order.) As is well known, the simplest atoms, the hydrogen-like atom with only one electron, exhibits higher degeneracies than one would expect from rotational and parity symmetry alone. Thus, the non-relativistic energy levels depend on the main quantum number $n$ alone. If we instead treat the problem relativistically with the Dirac equation replacing the non-relativistic Schrödinger equation, we again obtain higher degeneracies than expected. In the latter case the energy levels depend only on the total angular momentum $j$ but not on the parity. Thus the 2s state and the 2p state with $j=\frac{1}{2}$ are degenerate. The degeneracy is lifted by a small radiative correction $\Delta$, about a tenth of the already small difference between the 2p states with $j=1/2$ and $j=3/2$ (about $10^{-4}$ eV for the H atom).

## Appendix A

In this Appendix we want to verify that

$$\frac{1}{x+i\eta} \to \frac{P}{x} - i\pi\delta(x) \tag{A1}$$

when $\eta \to 0$. We choose an arbitrary but smooth test function $g(x)$ and an arbitrary positive number $\varepsilon$. In the limit when $\eta$ is much smaller than $\varepsilon$ we have

$$I(g,\eta) \equiv \int dx\, \frac{g(x)}{x+i\eta} = \int_{|x|>\varepsilon} \frac{g(x)}{x} + \int_{|x|<\varepsilon} \frac{g(x)}{x+i\eta}\,.$$

The first term can be made arbitralily close to a principal value integral by a suitable choice of $\varepsilon$. In the second term we can replace $g(x)$ by $g(0)$ if $\varepsilon$ was chosen small enough. The remaining integral tends to $-i\pi$. Since $g$ was arbitrary, this proves Eq. (A1).

## References

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