

Electron Self Energy Corrections

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If one calculates the energy of a point charge using classical electromagnetism, the result is infinite, yet as far as we know, the electron is point charge. One can calculate the energy needed to assemble an electron due, essentially, to the interaction of the electron with its own field. A uniform charge distribution with the classical radius of an electron, we have an energy $m_e c^2$. Experiments have probed the electron's charge distribution and found that it is consistent with a point charge down to distances much smaller than the classical radius. Beyond classical calculations, the self energy of the electron calculated in the quantum theory of Dirac is still infinite but the divergences are less severe.

At this point we must take the unpleasant position (constant) infinite energy should just be subtracted when we consider the overall zero of energy (as we did for the field energy in the vacuum). Electrons exist and don't carry infinite amount of energy baggage so we just subtract off the infinite constant. Nevertheless, we will find that the electron's self energy may change when it is a bound state and we should account for this change in our energy level calculations. This calculation will also give us the opportunity to understand resonant behaviour in scattering.

We can calculate the lowest order self energy corrections represented by the two Feynman diagrams below.



In these, a photon is emitted then reabsorbed. As we now know, both of these amplitudes are in order e^2 . The first one comes from the A^2 term in which the number of photons changes by zero or two and the second comes from the $\vec{A} \cdot \vec{p}$ term in second order time dependent perturbation theory. A calculation of the first diagram will give the same result for a free electron and a bound electron, while the second diagram will give different results because the intermediate states are different if an electron is bound than they are if it is free. We will therefore compute the amplitude from the second diagram.

$$H_{\text{int}} = -\frac{e}{mc} \vec{A} \cdot \vec{p}$$

$$\vec{A} = \frac{1}{\sqrt{V}} \sum_{\vec{k}, \alpha} \sqrt{\frac{\hbar c^2}{2\omega}} \hat{\epsilon}^{(\alpha)} \left(a_{\vec{k}, \alpha} e^{i(\vec{k} \cdot \vec{x} - \omega t)} + a_{\vec{k}, \alpha}^\dagger e^{-i(\vec{k} \cdot \vec{x} - \omega t)} \right).$$

This contains a term causing absorption of a photon and another term causing emission. We separate the terms for absorption and emission and pull out the time dependence.

$$\mathbf{H}_{\text{int}} = \sum_{\vec{k}, \alpha} \left(H_{\vec{k}, \alpha}^{\text{abs}} e^{-i\omega t} + H_{\vec{k}, \alpha}^{\text{emit}} e^{i\omega t} \right)$$

$$\mathbf{H}^{\text{abs}} = -\sqrt{\frac{\hbar e^2}{2m^2 \omega V}} a_{\vec{k}, \alpha} e^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)}$$

$$\mathbf{H}^{\text{emit}} = -\sqrt{\frac{\hbar e^2}{2m^2 \omega V}} a_{\vec{k}, \alpha}^\dagger e^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)}.$$

The initial and final state is the same $|n\rangle$, and second order perturbation theory will involve a sum over intermediate, and second order perturbation theory will involve a sum over intermediate atomic states, $|j\rangle$ and photon states. We will use the matrix elements of the interaction Hamiltonian between those states.

$$\begin{aligned}\mathbf{H}_{jn} &= \langle j | \mathbf{H}_{\vec{k},\alpha}^{\text{emit}} | n \rangle \\ \mathbf{H}_{nj} &= \langle n | \mathbf{H}_{\vec{k},\alpha}^{\text{abs}} | j \rangle \\ \mathbf{H}_{nj} &= \mathbf{H}_{jn}^*.\end{aligned}$$

In this case, we want to use the equations for the state we are studying, ψ_n , and all intermediate states, ψ_j plus a photon. Transitions can be made by emitting a photon from ψ_n to an intermediate state and transitions can be made back to the state ψ_n from any intermediate state. We neglect transitions from one intermediate state to another as they are higher order. (The diagram is emit a photon from ψ_n then reabsorb it.) The differential equations for the amplitudes are then.

$$\begin{aligned}i\hbar \frac{dc_j}{dt} &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} e^{i\omega t} c_n e^{i\omega_{nj}t} \\ i\hbar \frac{dc_n}{dt} &= \sum_{\vec{k},\alpha} \sum_j \mathbf{H}_{nj} e^{i\omega t} c_j e^{i\omega t}.\end{aligned}$$

In the equations for c_n , we explicitly account for the fact that an intermediate state can make a transition back to the initial state. Transitions through another intermediate state would be higher order and thus should be neglected. Note that the matrix elements for the transitions to and from the initial state are closely related. We also include the effect that the initial state can become depleted as intermediate states are populated by using c_n (instead of 1) in the equation for c_j . Note also that all the photon states will make nonzero contributions to the sum.

Our task is to solve these coupled equations. Previously, we did this by integration, but needed the assumption that the amplitude to be in the initial state was 1. Since we are attempting to calculate an energy shift, let us make that assumption and plug it into the equations to verify the solution.

$$c_n = e^{\frac{-i\Delta E_n t}{\hbar}} \quad (1)$$

ΔE_n will be a complex number, the real part of which represents an energy shift, and the imaginary part of which represents the lifetime (and energy width) of the state.

$$\begin{aligned}i\hbar \frac{dc_j}{dt} &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} e^{i\omega t} c_n e^{-i\omega_{nj}t} \\ c_n &= e^{\frac{-i\Delta E_n t}{\hbar}} \\ c_j(t) &= \frac{1}{i\hbar} \sum_{\vec{k},\alpha} \int_0^t dt' \mathbf{H}_{jn} e^{i\omega t'} e^{\frac{-i\Delta E_n t'}{\hbar}} e^{-i\omega_{nj}t'} \\ c_j(t) &= \frac{1}{i\hbar} \sum_{\vec{k},\alpha} \int_0^t dt' \mathbf{H}_{jn} e^{i(-\omega_{nj}-\Delta\omega_n+\omega)t'} \\ c_j(t) &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} \left[\frac{e^{i(-\omega_{nj}-\Delta\omega_n+\omega)t'}}{\hbar(\omega_{nj} + \Delta\omega_n - \omega)} \right]_0^t \\ c_j(t) &= \sum_{\vec{k},\alpha} \mathbf{H}_{jn} \frac{e^{i(-\omega_{nj}-\Delta\omega_n+\omega)t-1}}{\hbar(\omega_{nj} + \Delta\omega_n - \omega)}.\end{aligned}$$

Substitute this back into the differential equation for c_n to verify the solution and to find out what ΔE_n is. Note that the double sum over photons reduces to a single sum because we must absorb the same type of photon that

was emitted. (We have not explicitly carried along the photon state for economy.)

$$\begin{aligned}
i\hbar \frac{dc_n}{dt} &= \sum_{\vec{k}, \alpha} \sum_j \mathbf{H}_{nj} e^{-i\omega t} c_j e^{i\omega_{nj} t} \\
c_j(t) &= \sum_{\vec{k}, \alpha} \mathbf{H}_{jn} \frac{e^{i(-\omega_{nj} - \Delta\omega_n + \omega)t} - 1}{\hbar (\omega_{nj} + \Delta\omega_n - \omega)} \\
i\hbar \frac{dc_n}{dt} &= \Delta E_n e^{-i\Delta E_n t/\hbar} = \sum_{\vec{k}, \alpha} \sum_j \mathbf{H}_{nj} \mathbf{H}_{jn} e^{-i\omega t} e^{i\omega_{nj} t} \frac{e^{i(-\omega_{nj} - \Delta\omega_n + \omega)t} - 1}{\hbar (\omega_{nj} + \Delta\omega_n - \omega)} \\
\Delta E_n &= \sum_{\vec{k}, \alpha} \sum_j |\mathbf{H}_{nj}|^2 e^{i(\omega_{nj} + \Delta\omega_n - \omega)t} \frac{e^{i(-\omega_{nj} - \Delta\omega_n + \omega)t} - 1}{\hbar (\omega_{nj} + \Delta\omega_n - \omega)} \\
\Delta E_n &= \sum_{\vec{k}, \alpha} \sum_j |\mathbf{H}_{nj}|^2 \frac{1 - e^{i(\omega_{nj} + \Delta\omega_n - \omega)t}}{\hbar (\omega_{nj} + \Delta\omega_n - \omega)}.
\end{aligned}$$

Since this is a calculation to order e^2 and the interaction Hamiltonian squared contains a factor of e^2 we should drop the $\Delta\omega_n = \Delta E_n/\hbar$ s from the right hand side of this equation.

$$\Delta E_n = \sum_{\vec{k}, \alpha} \sum_j |\mathbf{H}_{nj}|^2 \frac{1 - e^{i(\omega_{nj} - \omega)t}}{\hbar (\omega_{nj} - \omega)} \quad (2)$$

We have a solution to the coupled differential equations to order e^2 . We should let $t \rightarrow \infty$ since the self energy is not a time dependent thing, however, the result oscillates as a function of time. This has been the case for many of our important delta functions, like the dot product of states with definite momentum. Let us analyze this self energy expression for large time.

We have something of the form.

$$-i \int_0^t e^{ixt'} dt' = \frac{1 - e^{ixt}}{x} \quad (3)$$

If we think of x as a complex number, our integral goes along the real axis. In the upper half plane, just above the real axis, $x \rightarrow x + i\epsilon$, the function goes to zero at infinity. In the lower half plane it blows up at infinity and on the axis, it's not well defined. We will calculate our result in the upper half plane and take the limit as we approach the real axis.

$$\lim_{t \rightarrow \infty} \frac{1 - e^{ixt}}{x} = \lim_{\epsilon \rightarrow 0+} i \int_0^\infty e^{ixt'} dt' = \lim_{\epsilon \rightarrow 0+} \frac{1}{x + i\epsilon} = \lim_{\epsilon \rightarrow 0+} \left[\frac{x}{x^2 + \epsilon^2} - \frac{i\epsilon}{x^2 + \epsilon^2} \right] \quad (4)$$

This is well behaved everywhere except at $x = 0$. The second term goes to $-\infty$ there. A little further analysis could show that the second term is a delta function.

$$\lim_{t \rightarrow \infty} \frac{1 - e^{ixt}}{x} = \frac{1}{x} - i\pi\delta(x) \quad (5)$$

Recalling that $c_n e^{-iE_n t/\hbar} = e^{-\frac{i\Delta E_n t}{\hbar}} e^{-iE_n t/\hbar} = e^{-i(E_n + \Delta E_n)t/\hbar}$, the real part of ΔE_n corresponds to an energy shift in the state $|n\rangle$ and the imaginary part corresponds to a width.

$$\begin{aligned}
\Re(\Delta E_n) &= \sum_{\vec{k}, \alpha} \sum_j \frac{|\mathbf{H}_{nj}|^2}{\hbar (\omega_{nj} - \omega)} \\
\Im(\Delta E_n) &= -\pi \sum_{\vec{k}, \alpha} \sum_j \frac{|\mathbf{H}_{nj}|^2}{\hbar} \delta(\omega_{nj} - \omega) = -\pi \sum_{\vec{k}, \alpha} \sum_j |\mathbf{H}_{nj}|^2 \delta(E_n - E_j - \hbar\omega).
\end{aligned}$$

All photon energies contribute to the real part. Only photons that satisfy the delta function constraint to the imaginary part. Moreover, there will only be an imaginary part if there is a lower energy state into which the state in question can decay. We can relate this width to those we previously calculated.

$$-\frac{2}{\hbar} \Im (\Delta E_n) = \sum_{\vec{k}, \alpha} \sum_j \frac{2\pi |\mathbf{H}_{nj}|^2}{\hbar} \delta(E_n - E_j - \hbar\omega) \quad (6)$$

The time dependence of the wavefunction for the state n is modified by the self energy correction.

$$\psi_n(\vec{x}, t) = \psi_n(\vec{x}) e^{-i(E_n + \Re(\Delta E_n))t/\hbar} e^{-\frac{\Gamma_n t}{2}} \quad (7)$$

This also gives us the exponential decay behaviour that we expect, keeping resonant scattering cross sections from going to infinity. So, the width just goes into the time dependence as expected and we don't have to worry about it anymore. We can now concentrate on the energy shift due to the real part of ΔE_n .

$$\begin{aligned} \Delta E_n &\equiv \Re(\Delta E_n) = \sum_{\vec{k}, \alpha} \sum_j \frac{|\mathbf{H}_{nj}|^2}{\hbar(\omega_{nj} - \omega)} \\ \mathbf{H}_{nj} &= \langle n | \mathbf{H}_{\vec{k}, \alpha}^{\text{abs}} | j \rangle \\ \mathbf{H}^{\text{abs}} &= -\sqrt{\frac{\hbar e^2}{2m^2 \omega V}} E^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)} \\ \Delta E_n &= \frac{\hbar e^2}{2m^2 V} \sum_{\vec{k}, \alpha} \sum_j \frac{\left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)} | j \rangle \right|^2}{\hbar \omega (\omega_{nj} - \omega)} \\ &= \frac{e^2}{2m^2 V} \int \frac{V d^3 k}{(2\pi)^3} \sum_{\alpha} \sum_j \frac{\left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)} | j \rangle \right|^2}{\omega (\omega_{nj} - \omega)} \\ &= \frac{e^2}{(2\pi)^3 2m^2} \sum_{\alpha} \sum_j \int d\Omega \frac{k^2 dk}{\omega} \frac{\left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} \cdot \hat{\epsilon}^{(\alpha)} | j \rangle \right|^2}{(\omega_{nj} - \omega)} \\ &= \frac{e^2}{(2\pi)^3 2m^2 c^3} \sum_j \sum_{\alpha} \int d\Omega \int \frac{\omega \left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} | j \rangle \cdot \hat{\epsilon}^{(\alpha)} \right|^2}{(\omega_{nj} - \omega)} d\omega. \end{aligned}$$

In our calculation of the total decay rate summed over polarization and integrated over photon direction we computed the cosine of the angle between each polarization vector and the (vector) matrix element. Summing these two and integrating over photon direction we got a factor of $\frac{8\pi}{3}$ and the polarization is eliminated from the matrix element. The same calculation applies here.

$$\begin{aligned} \Delta E_n &= \frac{e^2}{(2\pi)^3 2m^2 c^3} \sum_j \frac{8\pi}{3} \int \frac{\omega \left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} | j \rangle \right|^2}{(\omega_{nj} - \omega)} d\omega \\ &= \frac{e^2}{6\pi^2 m^2 c^3} \sum_j \int \frac{\omega \left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} | j \rangle \right|^2}{(\omega_{nj} - \omega)} d\omega \\ &= \frac{2\alpha \hbar}{3\pi m^2 c^2} \sum_j \int \frac{\omega \left| \langle n | e^{i\vec{k} \cdot \vec{x}} \vec{p} | j \rangle \right|^2}{(\omega_{nj} - \omega)} d\omega. \end{aligned}$$

Note that we wish to use the electric dipole approximation which is not valid for large $k = \frac{\omega}{c}$. It is valid up to about 2000 eV so we wish to cut off the calculation around there. While this calculation clearly diverges,

things are less clear here because of the eventually rapid oscillation of the $e^{i\vec{k}\cdot\vec{x}}$ term in the integrand as the E1 approximation fails. Nevertheless, the largest differences in corrections between free electrons and bound electrons occur in the region in which the E1 approximation is valid. For now we will just use it and assume the cut-off is low enough.

It is the difference between the bound electron's self energy and that for a free electron in which we are interested. Therefore, we will start with the free electron with a definite momentum \vec{p} . The normalized wave function for the free electron is $\frac{1}{\sqrt{V}}e^{i\vec{p}\cdot\vec{x}}/\hbar$.

$$\begin{aligned}
\Delta E_{\text{free}} &= \frac{2\alpha\hbar}{3\pi m^2 c^2 V^2} \sum_{\vec{p}'} \int \frac{\omega}{(\omega_{nj} - \omega)} \left| \int e^{-i\vec{p}\cdot\vec{x}/\hbar} \vec{p} e^{i\vec{p}'\cdot\vec{x}/\hbar} d^3x \right|^2 d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2 V^2} |\vec{p}|^2 \sum_{\vec{p}} \int \frac{\omega}{(\omega_{nj} - \omega)} \left| \int e^{i(\vec{p}'/\hbar - \vec{p}/\hbar)\cdot\vec{x}} d^3x \right|^2 d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2 V^2} |\vec{p}|^2 \sum_{\vec{p}'} \int \frac{\omega}{(\omega_{nj} - \omega)} |V \delta_{\vec{p}', \vec{p}}|^2 d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2} |\vec{p}|^2 \int_0^\infty \frac{\omega}{(\omega_{nj} - \omega)} d\omega \\
&= \frac{2\alpha\hbar}{3\pi m^2 c^2} |\vec{p}|^2 \int_0^\infty \frac{\omega}{(\omega_{nj} - \omega)} d\omega \rightarrow -\infty.
\end{aligned}$$

It's easy to see that this will go to negative infinity if the limit on the integral is infinite. It is quite reasonable to cut off the integral at some energy beyond which the theory we are using is invalid. Since we are still using non-relativistic quantum mechanics, the cut-off should have $\hbar\omega \ll mc^2$. For the E1 approximation, it should be $\hbar\omega \ll 2\pi\hbar c/1 = 10keV$. We will approximate $\frac{\omega}{(\omega_{nj} - \omega)} \approx -1$ since the integral is just giving us a number and we are not interested in high accuracy here. We will be more interested in accuracy in the next section when we compute the difference between free electron and bound electron self energy corrections.

$$\Delta E_{\text{free}} = \frac{2\alpha\hbar}{3\pi m^2 c^2} |\vec{p}|^2 \int_0^{E_{\text{cut}} - \text{off}/\hbar} \frac{\omega}{(\omega_{nj} - \omega)} d\omega.$$