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MASTER THESIS

Quasipotential approach to the Bethe-Salpeter equation for positronium

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Chapter 1 Introduction

This work is concerned with outlining a method of calculating energies of bound states in quantum field theories. However, before moving on to explaining the method itself, we would like to take a moment to motivate it. We will do so by answering some questions that the reader may have, starting with the most natural one: why study bound states in the first place?

Why study bound states?

First of all, there is a purely theoretical motivation for studying bound states – the setup of quantum field theory was motivated by scattering problems, and bound states present us with a different approach to understanding it. As we will see, perturbation theory in its usual sense cannot apply to bound state physics, because of the implicit assumption that the interaction energy in a process is much smaller than the kinetic energy. Because of this, a different sort of perturbation theory has to be developed, leading to a better understanding of the theory.

Secondly, a vast majority of objects available for experimental study are in fact bound states. An atom, a nucleus of an atom, a meson or baryon are all sources of empirical information to check the respective theories describing them. In fact historically, the hydrogen atom was at the center of theory development, ever higher precision of experiments revealing first the fine, later the hyperfine structure and the Lamb shift. All of these quantities can now be measured to an extremely high precision not only in hydrogen, but in other exotic atoms such as positronium (e^+e^- bound state) and muonium (μ^+e^- bound state, the $\mu^+\mu^$ state is called "true muonium"), providing us with precision tests of the validity of QED. The energy splittings and decay rates of these atoms can be explained within QED, without adding any additional parameters, and the theoretical predictions are largely in agreement with experiment, though there still are some problems. The situation is worse in QCD, where all observable particles are almost by definition bound states. As of yet, there is no calculation of meson masses from first principles, without addition of any new parameters to the theory – a problem closely related to understanding confinement in QCD. Which brings us to the next question...

Why study them in field theory rather than quantum mechanics?

Apart from the obvious need for higher precision calculations in hydrogen-like atoms, that cannot be met by quantum mechanics, there are other reasons to study bound states in field theory. Consider heavy quarkonia, which are predominantly non-relativistic. There is a well known similarity between the spectra of heavy quarkonia and that of positronium, motivating the use of the Cornell potential to describe mesons. Attempts have been made to construct a quantum mechanical quark model to explain the energy splittings in charmonia, however this type of models suffers from a high number of free parameters, originating from the potential that has to be postulated ad-hoc. Moreover, despite the number of parameters, the precision of predictions is far from accurate by QED standards. This naturally raises a question: can this potential be obtained directly from QCD by making a suitable approximation? There are attempts to do this too, though only partially successful. Even though the number of parameters is reduced, the confinement potential is still put in by hand, thus reducing the overall reliability of the method. Another common issue that models of this sort have, is the disagreement between the free quark mass and the constituent quark mass. Even though it is understood that quarks in mesons are "dressed" and their mass as appearing in the model need not be the same as the free mass, in principle there is no reason why the constituent mass should be impossible to calculate from first principles. Rather, this is a downfall of these types of models, that simply have the constituent mass as a parameter.

Aside from proper understanding of meson masses, recent discoveries of states that do not fit into the conventional quark model also call for a consistent treatment of bound states. In order to understand whether a given particle is a charmonium state, or a meson molecule, or a tetraquark, one obviously needs a reliable field theoretical description of bound states.

Why positronium?

The method we outline is quite general and can in principle be applied to any theory (granted that the system is mostly non-relativistic). However, in order to demonstrate it we have picked a particular example to work with – computing the hyperfine splitting in positronium. There are several reasons for doing that. The first one being the isolated nature of the problem – positronium to a very high degree of precision is purely electrodynamic, unlike for instance hydrogen, where the size of the proton starts playing a role at some point. This lets us work with QED, without adding any additional assumptions. Therefore the precision of the calculation rests on the validity of the method, rather than the theory itself – something that would not be possible if we worked on a problem in nuclear physics for instance, where the approximations done in the process of establishing the effective theory would also need to be questioned after obtaining the result.

Another reason is the abundance and precision of experimental data on positronium, something that would not be available had we chosen to work on exotic mesons, for instance.

Lastly, positronium is a two body problem, the simplest case for bound states. We will discuss possible applications of this method to three body problems at the end of this work.

Chapter 2

Propagator

2.1 The Propagator as a Green's Function

Although the discussion in this section applies to propagators of any theory, here we will focus on a particular example for clarity. We will consider a massive scalar field with the familiar Lagrangian:

$$\mathcal{L} = \frac{1}{2}\phi\,\partial^{\mu}\partial_{\mu}\phi - \frac{1}{2}m^{2}\phi^{2} + \mathcal{L}_{int}.$$
(2.1.1)

Why is the 2-point Green's function (GF) called the propagator? Written out explicitly:

$$\Delta(x_2 - x_1) = \langle \Omega | T\phi(x_1)\phi(x_2) | \Omega \rangle.$$
(2.1.2)

Since the theory is translation invariant, the expectation value may only depend on the coordinate difference. Assuming $t_2 > t_1$:

$$\Delta(x_2 - x_1) = \langle \Omega | \phi(x_2) \phi(x_1) | \Omega \rangle, \qquad (2.1.3)$$

which is the analogue of $\langle \vec{x}(t_2) | \vec{x}(t_1) \rangle$ in quantum mechanics. So the 2-point GF may be interpreted as the amplitude of a particle propagating from position \vec{x}_1 to \vec{x}_2 within the time frame $t_2 - t_1$, hence the name – the propagator.

In an attempt to better understand the physical meaning of the propagator, let us first consider a particular case with $\mathcal{L}_{int} = 0$ – the free theory. We denote the propagator for this theory as Δ_0 . Of course because of translational invariance the propagator will not depend on both coordinates x_1 and x_2 , but rather on the relative coordinate $x_2 - x_1 \equiv x$. To make this explicit, let us shift the center of the coordinate system so that it coincides with x_1 , in which case $x'_2 = x$ and $x_1 = 0$. After this adjustment, it becomes obvious that the propagator only depends on x:

$$\Delta_0(x) = \langle 0|T\phi(x)\phi(0)|0\rangle.$$
(2.1.4)

If $x^0 \equiv t > 0$, $\phi(0)$ is going to act first, whereas if t < 0, then $\phi(x)$ acts first. We can express this using step functions:

$$\Delta_0(x) = \theta(t) \langle 0|\phi(x)\phi(0)|0\rangle + (1-\theta(t)) \langle 0|\phi(0)\phi(x)|0\rangle.$$
(2.1.5)

Now let us demonstrate that the propagator defined in this manner is also the GF of the Klein-Gordon equation (KGE). We have to prove the following equation holds:

$$(\partial^2 - m^2)\Delta_0(x) = i\delta(x). \tag{2.1.6}$$

(The factor of *i* may in principle be absorbed in the definition of the propagator, however we would rather keep it outside so that the propagator may later be generalized to an n-point GF.)Let us start by taking the time derivatives of $\Delta_0(x)$:

$$\partial_t \Delta_0(x) = \delta(t) \langle 0 | \phi(x) \phi(0) | 0 \rangle + \theta(t) \langle 0 | \partial_t \phi(x) \phi(0) | 0 \rangle - \delta(t) \langle 0 | \phi(0) \phi(x) | 0 \rangle + (1 - \theta(t)) \langle 0 | \phi(0) \partial_t \phi(x) | 0 \rangle.$$
(2.1.7)

One of the canonical commutation relations states that field operators at different space points commute at the same times. So since the $\delta(t)$ vanishes everywhere but at t = 0,

$$\delta(t) \langle 0 | [\phi(x), \phi(0)] | 0 \rangle = 0.$$
(2.1.8)

And $\partial_t \Delta_0(x)$ becomes:

$$\partial_t \Delta_0(x) = \theta(t) \langle 0 | \partial_t \phi(x) \phi(0) | 0 \rangle + (1 - \theta(t)) \langle 0 | \phi(0) \partial_t \phi(x) | 0 \rangle.$$
(2.1.9)

Taking one more time derivative:

$$\partial_t^2 \Delta_0(x) = \delta(t) \langle 0 | \partial_t \phi(x) \phi(0) | 0 \rangle + \theta(t) \langle 0 | \partial_t^2 \phi(x) \phi(0) | 0 \rangle - \delta(t) \langle 0 | \phi(0) \partial_t \phi(x) | 0 \rangle + (1 - \theta(t)) \langle 0 | \phi(0) \partial_t^2 \phi(x) | 0 \rangle.$$
(2.1.10)

This time we can use the second commutation relation, to show:

 $\delta(t)\langle 0|\left[\partial_t\phi(x),\phi(0)\right]|0\rangle = -i\delta(t)\delta(\vec{x}) = -i\delta(x)$ (2.1.11)

Computing the space derivative of $\Delta_0(x)$ is straightforward:

$$\nabla^2 \Delta_0(x) = \theta(t) \langle 0 | \nabla^2 \phi(x) \phi(0) | 0 \rangle + (1 - \theta(t)) \langle 0 | \phi(0) \nabla^2 \phi(x) | 0 \rangle.$$
(2.1.12)

Combining eq. (2.1.10), eq. (2.1.12) and the KGE for $\phi(x)$, we get:

$$-\partial_t^2 \Delta_0(x) + \nabla^2 \Delta_0(x) = i\delta(x) + \theta(t) \langle 0|(-\partial_t^2 + \nabla^2)\phi(x)\phi(0)|0\rangle + (1 - \theta(t)) \langle 0|\phi(0)(-\partial_t^2 + \nabla^2)\phi(x)|0\rangle$$
(2.1.13)
$$= i\delta(x) + m^2 \Delta_0(x)$$

And finally,

$$(\partial^2 - m^2)\Delta_0(x) = i\delta(x). \tag{2.1.14}$$

We have established that the propagator is the GF of the KGE. This means that if a source is added to the KGE, the solution of the resulting non-homogeneous KGE can be written down using the propagator $\Delta(x)$. Before doing that, however, we should solve eq. (2.1.14) for $\Delta_0(x)$ itself. We can achieve that by Fourier transforming the equation:

$$(-p^2 - m^2)\Delta_0(p) = i. (2.1.15)$$

We are tempted to immediately take the inverse Fourier transformation and write down the solution as:

$$\Delta_0(x) \stackrel{?}{=} \frac{-i}{(2\pi)^4} \int d^4p \, \frac{e^{ipx}}{p^2 + m^2}.$$
(2.1.16)

However, after taking a look at the rhs of this equation, we see that the integrand diverges when the particle goes on-shell at $p^2 = -m^2$. In what follows, we demonstrate the proper way to regularize this integral as well as provide an explanation for the fact that the propagator diverges when the particle goes on-shell.

2.2 The Feynman-Stueckelberg propagator and its poles

Let us see how the system behaves when we add the simplest interaction term to it, an interaction with a real outside source J(x):

$$\mathcal{L} = \frac{1}{2}\phi \,\partial^{\mu}\partial_{\mu}\phi - \frac{1}{2}m^{2}\phi^{2} + J\phi.$$
(2.2.1)

The equation of motion for this theory is the non-homogeneous KGE:

$$(\partial^2 - m^2)\phi(x) = -J(x).$$
 (2.2.2)

Since we have established that $\Delta_0(x)$ is the GF for this equation (though we still need to regularize eq. (2.1.14)!), we can write down the solution:

$$\phi(x) = \phi_0(x) - \int d^4y \, \frac{1}{i} \Delta_0(x-y) J(y), \qquad (2.2.3)$$

where $\phi_0(x)$ is the solution of the homogeneous KGE, and the second term,

$$\phi_J(x) \equiv \int d^4y \, i\Delta_0(x-y)J(y) \tag{2.2.4}$$

is the disturbance created by the source. Let us focus on this term, and see how the propagation of this disturbance is affected by the choice of the propagator regularization. Use eq. (2.1.16) to obtain:

$$\phi_J(x) \stackrel{?}{=} \frac{1}{(2\pi)^4} \int d^4y \, d^4p \, \frac{e^{ip(x-y)}}{p^2 + m^2} \, J(y). \tag{2.2.5}$$

Identifying the Fourier transformation of J(y), and splitting the integration variables:

$$\phi_J(x) \stackrel{?}{=} \frac{1}{(2\pi)^4} \int dp_0 \, d^3p \, \frac{e^{-ip_0 t} e^{i\vec{p}\cdot\vec{x}}}{-p_0^2 + \vec{p}^2 + m^2} \, J(p_0, \vec{p}\,) = \frac{1}{(2\pi)^4} \int d^3p \, e^{i\vec{p}\cdot\vec{x}} \int dp_0 \, \frac{e^{-ip_0 t}}{-p_0^2 + \vec{p}^2 + m^2} J(p_0, \vec{p}\,).$$
(2.2.6)

Assume for the moment that t > 0. In this case we can attempt to compute this integral in the complex plane, by completing the contour below the real axis. If the arc is parametrized by $p_0 = Re^{i\theta}$, $\theta \in [\pi, 2\pi]$, then the exponential on the arc is:

$$\exp(-ip_0 t) = \exp(-iR\cos\theta t)\exp(R\sin\theta t).$$
(2.2.7)

Since $\sin \theta < 0$ for this range of θ , as $R \to \infty$, the integral on the arc vanishes, and the contour integral reduces to the integral over the real axis. The same is true for t < 0 if we close the contour above the real axis this time.

For t > 0, the residue theorem then states that the result of the integral is:

$$\phi_J(t>0) \stackrel{?}{=} -\frac{2\pi i}{(2\pi)^4} \int d^3p \, e^{i\vec{p}\cdot\vec{x}} \sum_{p_0^*} e^{-ip_0^*t} \operatorname{Res} \Big\{ \frac{1}{-p_0^2 + \vec{p}^2 + m^2} J(p_0, \vec{p}\,) \Big\}, \tag{2.2.8}$$

where p_0^* are the poles of the integrand. The important thing to notice here is the following: the exponential factor $e^{-ip_0^*t}$ determines the late-time behaviour of the field disturbance. In particular, it is the pole that is closest to the real axis that has the slowest vanishing exponential, so it is the dominant contribution to the sum. Already, we can see that the poles of the propagator determine how source disturbances propagate at late times, however we are yet to identify said poles with physical particles of the theory.

Up until this point we have ignored the fact that the integrand has two poles on the contour of integration, which make the integral we are considering divergent:

$$p_0^* = \pm \sqrt{\vec{p}^2 + m^2} = \pm E(\vec{p}).$$
(2.2.9)

There are several different ways in which one can integrate around these poles, and ultimately, the deciding factor in the prescription we adapt should be the physical meaning of the results we obtain by shifting them in one manner or another.

Let us try to understand the effect of the following prescription:

$$\phi_J(t>0) \stackrel{?}{=} \frac{-2\pi i}{(2\pi)^4} \int d^3p \, e^{i\vec{p}\cdot\vec{x}} \sum_{p_0^*} e^{-ip_0^*t} \operatorname{Res} \Big\{ \frac{1}{-(p_0+i\epsilon)^2 + \vec{p}^2 + m^2} J(p_0,\vec{p}) \Big\}, \qquad (2.2.10)$$

the effect of which is simply shifting the two poles below the real axis by ϵ . Assuming that the source is sufficiently regular, the integral is evaluated as follows:

$$\phi_{J}(t>0) \stackrel{?}{=} \frac{-2\pi i}{(2\pi)^{4}} \int d^{3}p \, e^{i\vec{p}\cdot\vec{x}} \Big(e^{-i(E-i\epsilon)t} \lim_{p_{0}\to E-i\epsilon} \Big\{ -\frac{p_{0}-E+i\epsilon}{(p_{0}-E+i\epsilon)(p_{0}+E+i\epsilon)} J(p_{0},\vec{p}) \Big\} + e^{i(E+i\epsilon)t} \lim_{p_{0}\to -E-i\epsilon} \Big\{ -\frac{p_{0}+E+i\epsilon}{(p_{0}-E+i\epsilon)(p_{0}+E+i\epsilon)} J(p_{0},\vec{p}) \Big\} \Big),$$

$$(2.2.11)$$

and after taking the above limits:

$$\phi_J(t>0) \stackrel{?}{=} \frac{-2\pi i}{(2\pi)^4} \int \frac{d^3p}{2E} \left(-J(E,\vec{p})e^{i(\vec{p}\cdot\vec{x}-Et)} + J(-E,\vec{p})e^{i(\vec{p}\cdot\vec{x}+Et)} \right).$$
(2.2.12)

Now we would like to identify these plane waves for de Broglie waves for relativistic particles. We only expect to see the first term – it corresponds to a particle with momentum \vec{p} and energy $E(\vec{p}) = \sqrt{\vec{p}^2 + m^2}$. So in order to suppress the second term originating in the $p_0^* = -E(\vec{p})$ pole, instead of shifting the below the real axis, we shift it above the real axis. This results in the late ϕ_J :

$$\phi_J(t>0) = \frac{2\pi i}{(2\pi)^4} \int \frac{d^3p}{2E} J(E,\vec{p}) e^{i(\vec{p}\cdot\vec{x}-Et)}, \qquad (2.2.13)$$

and the early ϕ_J :

$$\phi_J(t<0) = \frac{2\pi i}{(2\pi)^4} \int \frac{d^3p}{2E} J(-E,\vec{p}) e^{i(\vec{p}\cdot\vec{x}+Et)}.$$
(2.2.14)

Doing this allows us to interpret the wave in eq. (2.2.14) as one corresponding to a particle with momentum $-\vec{p}$ and energy E, because the seemingly wrong sign in the evolution exponential arises because of considering negative times, that is propagating the field backwards in time. Now, if we reverse this "backward propagation", we get a particle with momentum $-\vec{p}$ being absorbed by a source, in contrast to what we see in eq. (2.2.13), where a particle of momentum \vec{p} is being emitted by the source. The above prescription of shifting the poles allows for a propagator that can describe bot of these processes.

This interpretation is due to Feynman and Stueckelberg, and the prescription required to shift the poles in the proper way is:

$$\Delta_0(x) = \frac{-i}{(2\pi)^4} \int dp^4 \frac{e^{ipx}}{p^2 + m^2 - i\epsilon}.$$
(2.2.15)

This manner of thinking also lets us interpret the poles at negative energy as antiparticles (absorbing a positron is the same as emitting an electron), but of course in this theory the distinction is quite artificial, and we would have to consider a complex field for a description containing particles and antiparticles with opposite charges.

We have established already in eq. (2.2.8) that the pole of the propagator closest to the real axis determines how fields behave at late times, allowing us to interpret the energy at which the pole occurs to be the energy (or if we are in the rest frame, the mass) of the particle corresponding to the field – of course this means that the propagator diverges when the field goes on-shell.

This is true in general for other GF's as well, but in a bit of a different way. We will see in section 3.2 that if incoming particles can form and propagate as a bound state, this also results in a pole in the GF. We will be interested only in two body bound states, so we only consider 4-point GFs, however this is true in general as we will show.

2.3 The propagator in an interacting theory

As we have seen in the previous section, at late times field disturbances look like plane waves, which allows us to associate them with their corresponding particles. However, there is an interesting point to be made here: plane waves propagate indefinitely – so the particle never decays. And yet, obviously, unstable particles exist, and we hope that field theory is able to predict their decay widths. So how is this instability indicated on the propagator?

For us to consider decaying particles, we have to abandon the free theory, since a particle obviously cannot decay if it does not interact with other particles. Of course computing the propagator in an interacting theory is also much harder, however we can make use of perturbation theory and the Dyson equation. In perturbation theory, we consider the propagator to be free initially, and add the corrections coming from interactions perturbatively. For instance, some of the loop diagrams contributing to the electron propagator in QED are shown on fig. 2.3.1.



Figure 2.3.1: Contributions to the full electron propagator.

The diagrams contributing to the propagator can be divided into two categories: the reducible ones and irreducible ones. An irreducible diagram is a diagram that cannot be reduced to two different diagrams by cutting a single electron line – the three top diagrams in fig. 2.3.1 are all examples of irreducible diagrams. Reducible diagrams, on the other hand, can always be cut into two or more irreducible diagrams – the two bottom diagrams in fig. 2.3.1 are reducible, and the dashed line indicates where they can be cut to be reduced.

All of the one-particle irreducible diagrams make up what is called the one-particle irreducible (**1PI**) kernel Σ . In general, the integrals corresponding to the loop diagrams contained in Σ tend to be divergent – the problem that is solved by renormalization. Assuming we have renormalized the theory by adding all of the appropriate counterterms to the Lagrangian, the propagator is going to be given by a series iterating Σ – the Dyson series:



Figure 2.3.2: The Dyson series.

In this way we also include the reducible diagrams in a systematic way, of course.

$$\Delta = \Delta_0 + \Delta_0 \Sigma \Delta_0 + \Delta_0 \Sigma \Delta_0 \Sigma \Delta_0 + \dots \tag{2.3.1}$$



Figure 2.3.3: The one-particle irreducible kernel Σ .

$$\Delta = \Delta_0 + \Delta_0 \Sigma \Delta \tag{2.3.2}$$

Equation (2.3.2) is the Dyson equation and is central to our treatment of bound states. In this case, the exact propagator is found to be:

$$\Delta = \frac{-i}{p^2 + m^2 + i\Sigma - i\epsilon} \tag{2.3.3}$$

As one can see, the presence of interactions shifts the propagator poles, as expected. The real part of $i\Sigma$ simply accounts for the change in mass due to self-energy, and shifts the pole such that it is at the physical (or renormalized) mass. So what happens if the kernel has an imaginary part? The pole is then shifted into the imaginary plane:

$$-p_0^{*2} + \vec{p}^2 + m_R^2 + i \operatorname{Im}(i\Sigma) = 0$$
(2.3.4)

Assuming that the imaginary part is much smaller than the real part, the positive pole is at:

$$p_0^* \approx E(\vec{p}) + i \frac{\mathrm{Im}(i\Sigma)}{2E(\vec{p})}$$
(2.3.5)

Let us now define

$$\Gamma(\vec{p}) = -\frac{\mathrm{Im}(i\Sigma)}{E(\vec{p})} \tag{2.3.6}$$

The reason for the minus sign in the definition will be clear soon. To understand the physical meaning of Γ , let us return to eq. (2.2.10), and see how the exponential in the integral behaves when $p_0^* \approx E - \frac{i}{2}\Gamma$:

$$\phi_J(t>0) = \frac{-2\pi i}{(2\pi)^4} \int d^3p \, e^{i\vec{p}\cdot\vec{x}} e^{-i(E-\frac{i}{2}\Gamma)t} \operatorname{Res} \left\{ \frac{1}{-p_0^2 + \vec{p}^2 + m^2 - i\epsilon} J(p_0, \vec{p}\,) \right\}.$$
(2.3.7)

The imaginary part of the pole position introduces a damping term to the wave:

$$\phi_J(t>0) \sim e^{-\frac{1}{2}\Gamma t},$$
 (2.3.8)

which is exactly what we expect for a decaying particle. We can then interpret this imaginary contribution as the decay width of the particle. Although we should mention that the factor is only damping as long as $\Gamma > 0$, and actually increases the wave amplitude if $\Gamma < 0$, so in a unitary theory Γ will be positive.

Chapter 3

The Bethe-Salpeter equation

3.1 Dyson equation for the 4-point GF

The above discussion can be generalized for higher order GF's, too. Since we will be mostly interested in two-body bound states, we will only consider 4-point GF's, or two-particle propagators. We denote the free theory GF by S and the interacting theory GF by G. Notice that since in the free theory there is no way for the particles to exchange momentum, S is only a function of two variables – either the two momenta p_1 and p_2 , or the total and relative momenta $P = p_1 + p_2$ and $k = p_2 - p_1$. Whereas G is really a function of three variables: the total momentum P, the initial relative momentum $q = p_2 - p_1$ and the final relative momentum $q' = p_4 - p_3$.

Diagrams contributing to the 4-point GF are shown on fig. 3.1.1. We can define the twoparticle irreducible (**2PI**) kernel analogously to the **1PI** kernel and write down the Dyson series relating G to S.



Figure 3.1.1: Diagrams that contribute to the 4-point GF

The **2PI** kernel is all of the diagrams that cannot be cut into two by cutting only one particle and one particle line, for which the sum of momenta is equal to the total momentum.

For instance, the diagrams on the top row of fig. 3.1.1 are irreducible diagrams, and the ones on the bottom are reducible, with the dashed line showing how they can be reduced. We call the sum of all **2PI** diagrams K, shown on fig. 3.1.2.



Figure 3.1.2: **2PI** diagrams

Now, using this decomposition we can again write the Dyson series such that all of the reducible diagrams are also included, as shown on fig. 3.1.3.



Figure 3.1.3: The Dyson series for the 4-point GF

Resulting in:

$$G(p_1, p_2; p_3, p_4) = S(p_1, p_2) + S(p_1, p_2)K(p_1, p_2; p_3, p_4)S(p_3, p_4) + \int dk_1 S(p_1, p_2)K(p_1, p_2; k_1, q_1)S(k_1, q_1)K(k_1, q_1; p_3, p_4)S(p_3, p_4) + \dots,$$
(3.1.1)

where $q_1 = p_1 + p_2 - k_1$. This equation can be rewritten in a way similar to eq. (2.3.2), only this time with a convolution instead of a multiplication:

$$G(p_1, p_2; p_3, p_4) = S(p_1, p_2) + \int dk_1 S(p_1, p_2) K(p_1, p_2; k_1, q_1) G(k_1, q_1; p_3, p_4)$$
(3.1.2)

In principle, these fields can also have spin, in which case the GF will also depend on 4 spin indices. The spin indices will also be convoluted in a similar way. Since equations become quite cumbersome with both the convolutions explicit, we generally suppress at least one of them. The notation we use is explained in Appendix A. Suppressing the integration over relative momenta, we can rewrite this in a compact way:

$$G = S + SKG \tag{3.1.3}$$

Which looks deceivingly simple, and very similar to eq. (2.3.2). However, one has to keep in mind this is actually an integral equation, which makes it much harder to solve.

However, for our purposes here we need not solve this equation. Rather we will take advantage of the fact that in the presence of a bound state which overlaps with the two particle state described by G, the GF exhibits a pole and factorizes.

3.2 Factorization of GF near a bound state

We have stated before that in the presence of a bound state, the GF exhibits a pole. We will consider a GF responsible for the scattering of $n - r \phi$ -particles into $r \phi$ -particles, which means we will assume

$$p \equiv p_1 + \dots + p_r = p_{r+1} + \dots + p_n$$
 (3.2.1)

And the momentum space n-point function then is:

$$G(p_1, \dots p_n) = \int dx_1 \dots dx_n e^{-ip_1 x_1} \dots e^{-ip_r x_r} e^{ip_{r+1} x_{r+1}} \dots e^{ip_n x_n}$$

$$\times \langle \Omega | T \phi(x_1) \dots \phi(x_n) | \Omega \rangle.$$
(3.2.2)

Of course, the particular GF we are considering should have some sort of relationship with the bound state – we do not expect positronium to show up as a pole in the GF describing the electron-neutron scattering, for instance. Let us try to make this criterion exact. Assume that there exists a single particle state $|\Psi\rangle$ of mass M. The way for it to be connected to this particular GF is for it to have a non-zero overlap with the fields:

$$\langle \Psi | T\phi(x_1) \cdots \phi(x_r) | \Omega \rangle \neq 0.$$
 (3.2.3)

The assumptions have been listed, so we can move on to the proof. Consider first the time ordering in eq. (3.2.2). Among all the possible time orderings of the *n* time variables present here, let us focus on the contribution coming from the following one:

$$\langle \Omega | T\phi(x_1) \cdots \phi(x_n) | \Omega \rangle = \theta(\min[t_1, \dots t_r] - \max[t_{r+1}, \dots t_n]) \\ \times \langle \Omega | T\{\phi(x_1) \cdots \phi(x_r)\} T\{\phi(x_{r+1}) \cdots \phi(x_n)\} | \Omega \rangle + \text{extras}$$

$$(3.2.4)$$

which corresponds to the ordering in which all of the first r times is larger than all of the remaining ones. We will omit the argument of the theta function going further. Now proceed by inserting a complete set of states between the two time orderings:

$$\langle \Omega | T\phi(x_1) \cdots \phi(x_n) | \Omega \rangle$$

$$= \sum_{\text{state}} \theta \langle \Omega | T\{\phi(x_1) \cdots \phi(x_r)\} | \text{state} \rangle \langle \text{state} | T\{\phi(x_{r+1}) \cdots \phi(x_n)\} | \Omega \rangle$$

$$+ \text{extras.}$$

$$(3.2.5)$$

Among all of the states, let us pick out the contribution of the single particle state $|\Psi\rangle$, and push everything else into the extra terms:

$$\langle \Omega | T\phi(x_1) \cdots \phi(x_n) | \Omega \rangle$$

$$= \theta \int \frac{d^3p}{(2\pi)^3} \frac{1}{2E_{\Psi}} \langle \Omega | T\{\phi(x_1) \cdots \phi(x_r)\} | \Psi \rangle \langle \Psi | T\{\phi(x_{r+1}) \cdots \phi(x_n)\} | \Omega \rangle$$

$$+ \text{extras.}$$

$$(3.2.6)$$

In each of the time orderings we can pick one of the coordinates to measure all the other ones with respect to that one. Let us pick x_1 in the first set and x_{r+1} in the second one. Now we can rewrite $\phi(x_2)$ for example:

$$\phi(x_2) = e^{-i\hat{P}x_1}\phi(x_2 - x_1)e^{i\hat{P}x_1}.$$
(3.2.7)

Rewriting every field in this manner, and defining $x'_j \equiv x_j - x_1$ for j = 1, 2, ... r:

$$\begin{split} \left\langle \Omega \left| T\{\phi(x_1)\cdots\phi(x_r)\} \right| \Psi \right\rangle &= \left\langle \Omega \right| T\{e^{-i\hat{P}x_1}\phi(0)e^{i\hat{P}x_1}e^{-i\hat{P}x_1}\phi(x_2')e^{i\hat{P}x_1}\cdots e^{-i\hat{P}x_1}\phi(x_r')e^{i\hat{P}x_1}\} \left| \Psi \right\rangle \\ &= \left\langle \Omega \right| T\{\phi(0)\phi(x_2')\cdots\phi(x_r')\} \left| \Psi \right\rangle e^{ip_\Psi x_1} \end{split}$$

Similarly, defining $x'_j \equiv x_j - x_{r+1}$ for $j = r + 1, r + 2, \dots n$:

$$\langle \Psi | T\{\phi(x_{r+1})\cdots\phi(x_n)\} | \Omega \rangle = e^{-ip_{\Psi}x_{r+1}} \langle \Psi | T\{\phi(0)\cdots\phi(x'_n)\} | \Omega \rangle$$
(3.2.8)

Now let us go back to eq. (3.2.2) and change all of the integration variables to primed ones, except for x_1 and x_{r+1} :

$$G(p_{1}, ..., p_{n}) = \int dx_{1} dx'_{2} ... dx'_{r} dx_{r+1} dx'_{r+2} ... dx_{n} \times \\ \times e^{-ip_{1}x_{1}} ... e^{-ip_{r}(x'_{r}+x_{1})} e^{ip_{r+1}x_{r+1}} ... e^{ip_{n}(x'_{n}+x_{r+1})} \langle \Omega | \cdots | \Omega \rangle$$

$$= \int dx_{1} ... dx'_{n} e^{-i(p_{1}+...+p_{r})x_{1}} e^{i(p_{r+1}+...+p_{n})x_{r+1}} e^{-ip_{2}x'_{2}} ... e^{ip_{n}x'_{n}} \langle \Omega | \cdots | \Omega \rangle$$
(3.2.9)

Finally, we also have to change the variables in the argument of the theta function:

$$\min(t_1, \dots, t_r) = t_1 + \min(0, t'_2, \dots, t'_r)$$
$$\max(t_{r+1}, \dots, t_n) = t_{r+1} + \max(0, t'_{r+2}, \dots, t'_n)$$
$$\theta(\min[t_1, \dots, t_r] - \max[t_{r+1}, \dots, t_n]) = \theta(t_1 - t_{r+1} + \min[0, \dots, t'_r] - \max[0, \dots, t'_n]).$$

Use the integral representation of the theta function:

$$\theta(t) = \int \frac{d\omega}{2\pi} \frac{i}{\omega + i\epsilon} e^{-i\omega t}$$
(3.2.10)

Putting everything together:

$$G(p_1, \dots p_n) = \int \frac{d^3 p_{\Psi}}{(2\pi)^3} \frac{d\omega}{2\pi} dx_1 \dots dx'_n e^{-i(p_1 + \dots + p_r)x_1} e^{i(p_{r+1} + \dots + p_n)x_{r+1}} e^{-ip_2 x'_2} \dots e^{ip_n x'_n}$$

$$\times e^{-i\omega(t_1 - t_{r+1} + \min[0, \dots t'_r] - \max[0, \dots t'_n])} e^{ip_{\Psi} x_1} e^{-ip_{\Psi} x_{r+1}}$$

$$\times \frac{1}{2E_{\Psi}} \frac{i}{\omega + i\epsilon} \langle \Omega | T\{\phi(0)\phi(x'_2) \dots \phi(x'_r)\} | \Psi \rangle \langle \Psi | T\{\phi(0) \dots \phi(x'_n)\} | \Omega \rangle + \text{extras}$$

We can now take the x_1 and x_{r+1} integrals. Let us focus on the x_1 integral:

$$\int dt_1 d^3 x_1 e^{i(p_1^0 + \dots + p_r^0 - E_\Psi - \omega)t_1} e^{i(\vec{p}_\Psi - \vec{p}_1 - \dots - \vec{p}_r)\vec{x}_1} = (2\pi)^4 \delta(p_1^0 + \dots + p_r^0 - E_\Psi - \omega)\delta(\vec{p}_\Psi - \vec{p}_1 - \dots - \vec{p}_r).$$

Similarly, the integral over x_{r+1} will yield

$$(2\pi)^4 \delta(p_{r+1}^0 + \dots + p_n^0 - E_{\Psi} - \omega) \delta(\vec{p}_{\Psi} - \vec{p}_{r+1} - \dots - \vec{p}_n).$$
(3.2.11)

Take the p_{Ψ} integral:

$$G(p_1, \dots p_n) = \frac{(2\pi)^4 \delta(p_1 + \dots - p_n)}{2E_p} \int d\omega dx'_2 \dots dx'_n e^{-ip_2 x'_2} \dots e^{ip_n x'_n}$$

$$\times \delta(p_1^0 + \dots + p_r^0 - E_p - \omega) \frac{i}{\omega + i\epsilon} e^{-i\omega(t_1 - t_{r+1} + \min[0, \dots t'_r] - \max[0, \dots t'_n])} \quad (3.2.12)$$

$$\times \langle \Omega | T\{\phi(0)\phi(x'_2) \dots \phi(x'_r)\} | \Psi \rangle \langle \Psi | T\{\phi(0) \dots \phi(x'_n)\} | \Omega \rangle + \text{extras},$$

where $E_p = \sqrt{\vec{p}^2 + M^2}$. Since we are only interested in the pole around $\omega = 0$, we can set the argument in the exponential to zero, and take the ω integral:

$$G(p_1, \dots p_n) = (2\pi)^4 \delta(p_1 + \dots - p_n) \frac{i}{2E_p(p^0 - E_p + i\epsilon)}$$

$$\times \int dx'_2 \dots dx'_r \langle \Omega | T\{\phi(0)\phi(x'_2)\cdots\phi(x'_r)\} | \Psi \rangle \qquad (3.2.13)$$

$$\times \int dx'_{r+2} \dots dx'_n \langle \Psi | T\{\phi(0)\cdots\phi(x'_n)\} | \Omega \rangle + \text{extras}$$

Identify the last two lines with matrix elements $\mathcal{M}_{\Psi}^{1,r}$ and $\mathcal{M}_{\Psi}^{r+1,n\dagger}$, so that

$$G(p_1, \dots p_n) = (2\pi)^4 \delta(p_1 + \dots - p_n) \frac{i}{2E_p(p^0 - E_p + i\epsilon)} \mathcal{M}_{\Psi}^{1,r} \mathcal{M}_{\Psi}^{r+1,n\dagger} + \text{extras}$$
(3.2.14)

Notice that around the pole,

$$\frac{i}{2E_p(p^0 - E_p + i\epsilon)} = \frac{i}{2E_p(p^0 - E_p + i\epsilon)} \frac{p^0 + E_p}{p^0 + E_p}$$
$$= \frac{i}{(p^0)^2 - E_p^2 + i\epsilon}$$
$$= \frac{-i}{p^2 + M^2 - i\epsilon},$$

where we have redefined ϵ by absorbing a positive constant $p^0 + E_p$ into it.

$$G(p_1, \dots p_n) = (2\pi)^4 \delta(p_1 + \dots - p_n) \frac{-i}{p^2 + M^2 - i\epsilon} \mathcal{M}_{\Psi}^{1,r} \mathcal{M}_{\Psi}^{r+1,n\dagger} + \text{extras}$$
(3.2.15)

Hence the GF factorizes near the bound state pole: the matrix elements $\mathcal{M}_{\Psi}^{1,r}$ and $\mathcal{M}_{\Psi}^{r+1,n\dagger}$ only depend on the incoming or outgoing momenta (and any other degrees of freedom, such as spin) respectively. We now define the Bethe-Salpeter wavefunction in terms of these matrix elements as follows:

$$\Psi = \frac{\mathcal{M}_{\Psi}^{1,r}}{\sqrt{2E_p}} \qquad \bar{\Psi} = \frac{\mathcal{M}_{\Psi}^{r+1,n\dagger}}{\sqrt{2E_p}}, \qquad (3.2.16)$$

so that in the proximity of the bound state pole

$$G \to i \frac{\Psi(p_1 \cdots p_r)\Psi(p_{r+1} \cdots p_n)}{p^0 - E_p}.$$
 (3.2.17)

3.3 Bethe-Salpeter equation

Since the residue of the GF factorizes near the bound state pole, we can obtain an equation for the Bethe-Salpeter wavefunction from the Dyson equation. Comparing the residues on the two sides of eq. (3.1.3) for the case of the 4-point GF:

$$\Psi(p_1, p_2)\bar{\Psi}(p_3, p_4) = \int dk_1 S(p_1, p_2) K(p_1, p_2; k_1, q_1) \Psi(k_1, q_1) \bar{\Psi}(p_3, p_4), \qquad (3.3.1)$$

$$\Psi(p_1, p_2) = \int dk_1 S(p_1, p_2) K(p_1, p_2; k_1, q_1) \Psi(k_1, q_1), \qquad (3.3.2)$$

or schematically

$$\Psi = SK\Psi \tag{3.3.3}$$

One has to keep in mind that this equation only holds near the bound state pole, where $(p_1 + p_2)^2 = -M^2$. Equation (3.3.2) is known as the Bethe-Salpeter equation (BSE) [9].

We should mention that an equation for $\overline{\Psi}$ can also be obtained by resuming the Dyson equation in a different way

$$G = S + GKS, \tag{3.3.4}$$

which leads to the dual BSE

$$\bar{\Psi} = \bar{\Psi}KS. \tag{3.3.5}$$

Going forward we will only discuss eq. (3.3.3), but everything applies for the dual equation as well.

Chapter 4

The Quasipotential approach to BSE

4.1 Salpeter equation

The BSE is a four dimensional integral equation, with its kernel given by an infinite series in the coupling constant, which makes it extremely hard to solve. The first consistent approximation to this equation was developed by Salpeter [8]. Salpeter's approach involves replacing the exact kernel by its dominant part – the Coulomb interaction:

$$iK_C(\vec{p}) = -\frac{e^2}{|\vec{p}|^2} \gamma_0^{(1)} \gamma_0^{(2)}.$$
(4.1.1)

This approximate kernel is static, that is it has no energy dependence, which seems like it would simplify the equation, since one can now integrate the rhs of the equation over the relative energy. This is exactly how Salpeter proceeded, and obtained a three dimensional integral equation. It was possible to introduce retardation effects in this kernel, making the equation exact in principle. However, this zeroth order equation itself was not exactly solvable, forcing one to use perturbation theory to first obtain a zeroth order solution, and use more perturbation theory on top of it to get corrections to the Coulomb kernel. This was further complicated by the fact that the wavefunctions of the Salpter equation depend on the relative energy of constituents. All these problems combined make the scheme increasingly more awkward to apply for higher order corrections.

Another problem of the Salpeter equation we should mention is the wrong infinite mass limit. One would expect to recover the Dirac-Coulomb equation in the limit where the mass of one of the two constituents becomes infinite. But this is not the case for the Salpeter equation [6], which demonstrates a problem with the formalism. To be clear, one can actually recover the right infinite mass limit by including not only the Coulomb ladder diagrams, but also the crossed ladder diagrams. Obviously, this in itself complicates matters further.

The modern approach to approximating the BSE problem is more involved to account for all the problems researchers have encountered in the past. As the example of the Salpeter equation shows us, it is important to have a solvable zeroth order problem that already accounts for some of the reduced mass dependence. Further, it helps if the wavefunctions of the zeroth order problem do not depend on the relative energy of the constituents. Here we will present a variation of an approach satisfying these conditions, and use it to solve for energy levels of positronium in QED.

4.2 Reducing the BSE to the Schödinger-Coulomb equation

4.2.1 The freedom of propagator choice

Recall the Dyson equation for the renormalized 4-point GF:

$$G_R = S_R + S_R K_R G_R. aga{4.2.1}$$

We would like to reduce this equation to an exactly solvable three dimensional equation, without making approximations that cannot be accounted for in perturbation theory. There are several ways of doing that [1,2,6] which all rely on replacing the renormalized two particle propagator S_R by a simpler three dimensional propagator, which approximates its behaviour well in the non-relativistic regime – the regime appropriate for bound state calculations in positronium, muonium or hydrogen (some very early work in this area that lead to this approach was done by Logunov, Tavkhelidze and Faustov [7], [3]). For now we will not specify the exact form of the simplified propagator, but work with a generic one to demonstrate how the reduction happens.

Since we are changing the propagator, in order for the equation to remain exact, we have to somehow account for this change elsewhere. This is achieved by by adding compensating changes to the kernel in a way shown below.

$$G_R = S_0 + S_0 K G_R (4.2.2)$$

The K in eq. (4.2.2) has to be related to the K_R in eq. (4.2.1) in such a way that the GF resulting from the iteration does not change. Let us assume for now that S_0 has an inverse. Multiply eq. (4.2.1) by S_R^{-1} from the left, and eq. (4.2.2) by S_0^{-1} from the left to obtain:

$$S_R^{-1}G_R = 1 + K_R G_R$$

 $S_0^{-1}G_R = 1 + K G_R$.

It follows, that in order for eq. (4.2.2) to hold:

$$K = K_R + S_R^{-1} - S_0^{-1}, (4.2.3)$$

and indeed if the kernel is transformed in this way, eq. (4.2.2) and eq. (4.2.1) are equivalent.

The same can be done for the case where S_0 is not invertible, though it is somewhat harder to demonstrate. In order to show this we have to consider the truncated GF, defined below:

$$G_R = S_R + S_R G_T S_R, aga{4.2.4}$$

so that G_T is just the GF with the external propagators truncated. Rewriting eq. (4.2.1) in its explicit iterative form makes the explicit form of G_T clear:

$$G_R = S_R + S_R K_R S_R + S_R K_R S_R K_R S_R + \dots$$
$$G_T = K_R + K_R S_R G_T.$$

We now require that a similar equation holds for G_T with a different propagator and a transformed kernel.

$$G_T = K + K S_0 G_T \tag{4.2.5}$$

It can be explicitly shown that these equations hold if K is chosen in the following way:

$$K = K_R + K_R (S_R - S_0) K. (4.2.6)$$

Since we are choosing S_0 to approximate S_R as well as possible, the terms of higher order in $(S_R - S_0)$ are expected to be negligibly small, allowing us to approximate the transformed kernel by

$$K = K_R + K_R (S_R - S_0) K_R + \dots (4.2.7)$$

This is an important point that should be stressed: even though in principle the equation for G_T with a propagator of choice S_0 and a kernel transformed so as to fit this choice K is exact, there is in fact no hope to find an exact solution to this equation. Instead, what eq. (4.2.7) allows us to do is incorporate corrections (corrections due to a changed propagator) at any order of $(S_R - S_0)$ that we need to match experimental precision.

One can now go back to the untruncated GF, by attaching S_0 propagator legs to G_T . The resulting GF G is:

$$G = S_0 + S_0 G_T S_0. (4.2.8)$$

In this case, unlike in the case where S_0^{-1} exists, the GF resulting from a change of the propagator is not the same as G_R :

$$G \neq G_R. \tag{4.2.9}$$

However, if G were expressed in terms of G_R , we could check whether the bound state poles of these two GF's are the same. From eq. (4.2.4) and eq. (4.2.8):

$$G = S_0 + S_0 S_R^{-1} (G_R - S_R) S_R^{-1} S_0.$$
(4.2.10)

Since neither of the free two particle propagators S_R and S_0 can have bound state poles, it is clear from eq. (4.2.10) that G and G_R indeed have the same bound state poles.

In conclusion, irrespective of whether the propagator of choice S_0 is invertible or not, the renormalized two particle propagator can be replaced by S_0 , as long as a compensating transformation is performed on the kernel K_R . As stressed by Lepage [6], one is free to choose any two particle propagator that suits the problem at hand, precisely because of this fact.

4.2.2 Approximating the kernel

Let us assume we have chosen an S_0 , and the Dyson equation for G now has the following form:

$$G = S_0 + S_0 KG, (4.2.11)$$

where K is given by eq. (4.2.7) in terms of K_R , S_R and S_0 . By a suitable choice of S_0 this equation can be reduced to a three dimensional one, however another problem remains: K is given by a twofold infinite series. First of all it contains K_R – the two particle irreducible kernel given by an infinite series of diagrams with increasing powers of the coupling constant.

Secondly, it contains the terms of the type $K_R(S_R - S_0)K_R$, correcting for the change of the propagator. This difficulty is treated in the following manner: we pick the part of K that generates the dominant part of the bound state pole (we call this contribution K_0) and treat the rest of K in perturbation theory which we will outline in section 4.3.

Assuming we have picked K_0 as well, the Dyson equation becomes

$$G_0 = S_0 + S_0 K_0 G_0, (4.2.12)$$

where G_0 is the GF that results after this particular pick of K_0 . Let us name the bound state energies of G_0 as $\{E_n^0\}$, and those of G as $\{E_n\}$. These sets of energies will be related to each other by the perturbation theory in $\delta K = K - K_0$. In the case of hydrogen-like atoms in QED, the Coulomb exchange (or something that is approximately the Coulomb exchange) seems like a reasonable pick for K_0 . The Coulomb exchange will emerge in this framework as a part of the single photon exchange in K_R . In this case, we can immediately see that the simplest corrections contained in δK are:



Figure 4.2.1: Simplest contributions to δK .

And the simplest correction coming from $K_R(S_R - S_0)K_R$ would be:



Figure 4.2.2: Simplest contribution from $K_R(S_R - S_0)K_R$.

where we have replaced the full kernel K_R by single photon exchange.

Before discussing how exactly one calculates the shift in energy levels produced by these corrections, we will show how an appropriate choice of the propagator leads to the Schrödinger equation from eq. (4.2.12).

4.2.3 Motivation for a choice of S_0

Let us discuss the choice of the propagator. As we have mentioned before, there are many different ways of choosing S_0 , and each one is valid provided the kernel is transformed accordingly. We will use the choice of Bodwin, Yennie and Gregorio [2]. To make the

reason for this particular choice transparent, we need to re-parametrize the momenta of incoming and outgoing particles in terms of parameters more relevant to our problem. We will be concerned with two bound states in QED – positronium (e^+e^-) and muonium (μ^+e^-) , each of them consisting of a particle and an anti-particle. Let us call the momentum of the incoming (outgoing) electron $P_e(P'_e)$, and the momentum of the incoming (outgoing) positive anti-particle $P_p(P'_p)$. Re-parametrize them in a following way:

$$P_e^{\mu} = E' \delta_0^{\mu} + p^{\mu}, \quad P_p^{\mu} = E'' \delta_0^{\mu} - p^{\mu}$$
(4.2.13)

$$P^{\mu} = P^{\mu}_{e} + P^{\mu}_{p} = (E, \vec{0})$$
(4.2.14)

where P^{μ} is the total momentum and we are carrying out all our calculations in the rest frame of the bound state, so that E is the energy of the bound state. Since we know that both of these systems are highly non-relativistic and weakly bound, we expect each constituent of the bound state to be almost on its mass shell. This allows us to define

$$E'^2 = m_e^2 - \gamma^2, \quad E''^2 = m_p^2 - \gamma^2.$$
 (4.2.15)

Since the bound state is weakly bound, its energy E will be just below the total mass of the constituents $(m_e + m_p)$, so the energy of each constituent is just below its mass, too. This, combined with the fact that were the energy to be higher than the mass (like it is for scattering states), we would express E' and E'' in terms of relative momentum \vec{k} :

$$E'^2 = m_e^2 + \vec{k}^2, \quad E''^2 = m_p^2 + \vec{k}^2.$$
 (4.2.16)

It is exactly these considerations that inspire the definition in eq. (4.2.15). But ultimately, this is nothing but a re-parametrization, in which we replace the variable E by γ , since

$$E = E' + E'' = \sqrt{m_e^2 - \gamma^2} + \sqrt{m_p^2 - \gamma^2}.$$
(4.2.17)

Expressed in terms of E instead of γ , E' and E'' are

$$E' = \frac{E^2 - m_p^2 + m_e^2}{2E}, \quad E'' = \frac{E^2 + m_p^2 - m_e^2}{2E}.$$
(4.2.18)

Knowing that $\gamma^2 \ll m_e, m_p$, we can expand eq. (4.2.17) in powers of γ^2 , to get some insight into the physical meaning of γ :

$$E \approx m_e + m_p - \frac{\gamma^2}{2} \left(\frac{1}{m_e} + \frac{1}{m_p} \right).$$
 (4.2.19)

If we now define reduced mass as $m_r = m_e m_p / (m_e + m_p)$,

$$E \approx m_e + m_p - \frac{\gamma^2}{2m_r}.$$
(4.2.20)

Here, one can clearly see that the γ term in the energy is the binding energy. Just to get an estimate of how small γ is, let us consider the ground state solution of the Schrödinger-Coulomb equation with binding energy E_0^C :

$$E_0^C = -\frac{m_r \alpha^2}{2}.$$
 (4.2.21)

We deduce that γ is of the order $m_r \alpha$ for QED bound states, so it is indeed small compared to constituent masses, as expected.

The re-parametrization described above is usually referred to as momentum routing, and is in principle arbitrary. The way presented here treats the constituents symmetrically, however this need not be the case. For instance, Gross [4] puts one of the particles (the heavier one) on shell: E' = E - E'', $E'' = \sqrt{m_p^2 + \vec{k}^2}$. Even though the end result of the calculation cannot depend on momentum routing, the intermediate steps will, that is why it is important to choose one appropriate to the problem. If the problem at hand is positronium, it is more convenient to treat the two particles symmetrically, whereas if it is muonium or hydrogen, the asymmetric treatment might be more efficient.

We will start from the bare particle anti-particle propagator:

$$\Delta_0^{(1)}(P_e)\Delta_0^{(2)}(P_p) = \frac{-i(-\not\!\!P_e + m_e)^{(1)}}{P_e^2 + m_e^2 - i\epsilon} \frac{-i(\not\!\!P_p + m_p)^{(2)}}{P_p^2 + m_p^2 - i\epsilon}.$$
(4.2.22)

At this point we would like to explain the notation used to express this propagator. To make the explanation clear, let us consider a particular contribution to the GF – single photon exchange presented on fig. 5.3.2.



Figure 4.2.3: Single photon exchange contribution to the GF.

Evaluating this diagram, we get

single photon contr. =
$$\left[\Delta^{(1)}(P'_e)(ie\gamma_{\mu})\Delta^{(1)}(P_e)\right] \Delta^{\mu\nu} \left[\Delta^{(2)}(-P_p)(ie\gamma_{\nu})\Delta^{(2)}(-P'_p)\right], (4.2.23)$$

where $\Delta^{\mu\nu}$ is the photon propagator. Notice that the form in which a diagram would normally be evaluated does not fit the form of the Dyson equation: in the Dyson equation, this contribution has the form S(P, p)K(P, p, q)S(P, q), where S is the two particle propagator. However, in eq. (4.2.23) the single particle propagators appear on different sides of the equation. In the notation we use, this contribution would be rewritten as

single photon contr. =
$$\Delta^{(1)}(P_e)\Delta^{(2)}(P_p) \Big[\Big(ie\gamma_{\mu}^{(1)} \Big) \Delta^{\mu\nu} \Big(ie\gamma_{\nu}^{(2)} \Big) \Big] \Delta^{(1)}(P'_e)\Delta^{(2)}(P'_p)$$

= $S(P,p) \qquad K_{s.p.}(P,p,q) \qquad S(P,q).$ (4.2.24)

Notice that in the first line of eq. (4.2.24) we have kept the (1), (2) labels on the gamma matrices in the kernel, so that it is clear how to reconstruct eq. (4.2.23). Even though this

$$\Delta^{(1)}(P_e)\Delta^{(2)}(P_p) = \frac{-i(-\not\!\!P_e + m_e)^{(1)}}{P_e^2 + m_e^2 - i\epsilon} \otimes \frac{-i(\not\!\!P_p + m_p)^{(2)}}{P_p^2 + m_p^2 - i\epsilon}, \qquad (4.2.25)$$

however, we will refrain from using this notation here, as adding labels (1), (2) to matrices seems to be more self-evident.

We will always use the label (1) for the electron, and the label (2) for the anti-particle, be it a positron or an anti-muon.

Going back to the bare propagator in eq. (4.2.25), let use the momentum routing defined above to find a suitable approximation to it. For now, let us focus on the denominator of the equation:

$$\frac{1}{(E'\delta^{\mu}_{\ 0} + p^{\mu})^{2} + m_{e}^{2} - i\epsilon} \frac{1}{(E''\delta^{\mu}_{\ 0} - p^{\mu})^{2} + m_{p}^{2} - i\epsilon} = \frac{1}{\gamma^{2} + p^{2} - 2E'p^{0} - i\epsilon} \frac{1}{\gamma^{2} + p^{2} + 2E''p^{0} - i\epsilon}.$$
(4.2.26)

This expression can be split into a sum of two fractions in the following way:

$$= \frac{1}{2E} \frac{1}{\gamma^2 + p^2 - i\epsilon} \left[\frac{2E'}{\gamma^2 + p^2 - 2E'p^0 - i\epsilon} + \frac{2E''}{\gamma^2 + p^2 + 2E''p^0 - i\epsilon} \right].$$
(4.2.27)

Now focus on the expression in the brackets:

$$\left[\frac{1}{\frac{\gamma^2 + p^2}{2E'} - p^0 - i\epsilon} + \frac{1}{\frac{\gamma^2 + p^2}{2E''} + p^0 - i\epsilon}\right].$$
(4.2.28)

As we have stated before, in the case we are interested in, the binding energy (parametrized by $\gamma \sim \alpha m_r$) and the relative momentum are much less than the mass of the constituents. So since $E' \sim m_e$ and $E'' \sim m_p$, we may neglect the fractions in the denominators, to obtain:

$$\left[\frac{1}{-p^0 - i\epsilon} + \frac{1}{p^0 - i\epsilon}\right],\tag{4.2.29}$$

which is just a limit representation of the Dirac delta:

$$\lim_{\epsilon \to 0} \left[\frac{1}{-p^0 - i\epsilon} + \frac{1}{p^0 - i\epsilon} \right] = 2\pi i \delta(p^0).$$

$$(4.2.30)$$

Hence, in the non-relativistic regime the denominator of the propagator may be approximated by

$$2\pi i \,\frac{1}{2E} \,\frac{1}{\gamma^2 + p^2 - i\epsilon} \,\delta(p^0). \tag{4.2.31}$$

We would like to stress yet again that the approximations made here do not make the solution inexact, since as it was shown in previous sections, the choice of the propagator is arbitrary as long as it has the right behaviour in the non-relativistic regime. The procedure by which we find the propagator described here should be seen as a justification for our particular choice rather than a derivation.

For now the propagator is approximated by

$$\Delta_0^{(1)}(P_e)\Delta_0^{(2)}(P_p) \approx -2\pi i \frac{1}{2E} \frac{(-\not\!\!P_e + m_e)^{(1)}(\not\!\!P_p + m_p)^{(2)}}{\gamma^2 + \vec{p}^2 - i\epsilon} \,\delta(p^0), \qquad (4.2.32)$$

where we have set $p^0 = 0$ because of the Dirac delta. Let us now deal with the numerator structure of the propagator. We wish to split it into the part dominant in the non-relativistic regime, and the remainder.

$$(-E'\gamma_0 - p^i\gamma_i + m_e)^{(1)}(E''\gamma_0 - p^i\gamma_i + m_p)^{(2)} = \left(\left[\frac{1}{2}(E' + m_e)(1 - \gamma_0) \right] - \frac{1}{2}(E' - m_e)(1 + \gamma_0) - p^i\gamma_i \right)^{(1)} \times \left(\left[\frac{1}{2}(E'' + m_p)(1 + \gamma_0) \right] - \frac{1}{2}(E'' - m_p)(1 - \gamma_0) - p^i\gamma_i \right)^{(2)}$$

For each particle, the contribution in the square brackets dominates, and that is the part we keep for both particles.

$$\Delta_0^{(1)}(P_e)\Delta_0^{(2)}(P_p) \approx -2\pi i \,\frac{(E'+m_e)(E''+m_p)}{8E} \,\frac{(1-\gamma_0)^{(1)}(1+\gamma_0)^{(2)}}{\gamma^2+\vec{p}^2-i\epsilon} \,\delta(p^0). \tag{4.2.33}$$

This two particle propagator is what we will use in our analysis as S_0 :

$$S_0 \equiv -2\pi i \, \frac{(E'+m_e)(E''+m_p)}{4Em_r} \frac{1}{\frac{\gamma^2}{2m_r} + \frac{\vec{p}^2}{2m_r} - i\epsilon} \, \frac{(1-\gamma_0)^{(1)}}{2} \frac{(1+\gamma_0)^{(2)}}{2} \delta(p^0). \tag{4.2.34}$$

To simplify the derivation of the Schrödinger equation, we will present here a shorthand notation:

$$S_0 \equiv 2\pi i \,\delta(p^0) N \bar{s},\tag{4.2.35}$$

where we have defined

$$N \equiv \frac{(E'+m_e)(E''+m_p)}{4Em_r}, \qquad \bar{s} \equiv -\frac{1}{4} \frac{(1-\gamma_0)^{(1)}(1+\gamma_0)^{(2)}}{\frac{\gamma^2}{2m_r} + \frac{\vec{p}^2}{2m_r} - i\epsilon}.$$
 (4.2.36)

Notice that \bar{s} is proportional to the Schrödinger propagator, and the factor N is very close to unity, since $E' \approx m_e$, $E'' \approx m_p$ in the non-relativistic regime:

$$N \approx \frac{m_e m_p}{(m_e + m_p)m_r} = 1.$$
 (4.2.37)

Since we are free in the choice of the propagator, at first glance it seems that one can simply drop the factor of N, and just use the rest of the expression. However, as we have stated before having some of the reduced mass dependence accounted for in the propagator helps avoid spurious complications in the future calculations [2].

4.2.4 Emergence of the Schrödinger equation

Let us now use this propagator in the BSE. First, notice that the very first term of the expansion for the GF is simply the two particle propagator S_0 , yet since in the free theory particles cannot exchange momenta, we have to force p = q in this term. Taking this fact into account, the Dyson equation becomes:

$$G(P;p,q) = (2\pi)^4 \delta(p-q) S_0(P;p) + \int \frac{d^4k}{(2\pi)^4} S_0(P;p) K(P;p,k) G(P;k,q).$$
(4.2.38)

Now, impose $S_0(P;p) = 2\pi i \delta(p^0) N \bar{s}(\vec{p})$, and consider the open form of the Dyson equation:

$$G(P; p, q) = (2\pi)^4 \delta(p-q) S_0(P; p) + S_0(P; p) K(P; p, q) S_0(P; q) + S_0(P; p) K(P; p, k) S_0(P; k) K(P; k, q) S_0(P; q) + \dots$$

Notice that the first term can be rewritten as

$$\delta(p-q)\delta(p^0) = \delta(p^0)\delta(q^0)\delta(\vec{p}-\vec{q})$$
(4.2.39)

and each other term in the expansion contains S(P; p) and S(P; q), which means that every term will contain $\delta(p^0)\delta(q^0)$, such that we can rewrite G as

$$G(P; p, q) = (2\pi)^2 \bar{G}(P; \vec{p}, \vec{q}) \delta(p^0) \delta(q^0)$$
(4.2.40)

Using this expression in eq. (4.2.38):

$$\bar{G}(P;\vec{p},\vec{q}) = (2\pi)^3 i N \bar{s}(\vec{p}) + \int \frac{d^3k}{(2\pi)^3} N \bar{s}(\vec{p}) i \bar{K}(P;\vec{p},\vec{k}) \bar{G}(P;\vec{k},\vec{q}), \qquad (4.2.41)$$

where we have integrated over k^0 , and defined \bar{K} such that

$$\bar{K}(P;\vec{p},\vec{k}\,) = \lim_{p^0,k^0 \to 0} K(P;p,k).$$
(4.2.42)

The GF factorizes near a bound state pole at E_n :

$$G(P; p, q) \to i \frac{\Psi_n(p)\bar{\Psi}_n(q)}{E - E_n}$$
(4.2.43)

$$\bar{G}(P;\vec{p},\vec{q}) \to i \frac{\psi_n(\vec{p})\bar{\psi}_n(\vec{q})}{E - E_n}$$

$$(4.2.44)$$

Comparing the residues of the right side and the left side of eq. (4.2.41) at E_n , we obtain the modified BSE:

$$\psi_n(\vec{p}) = N\bar{s}(\vec{p}) \int \frac{d^3k}{(2\pi)^3} i\bar{K}(P;\vec{p},\vec{k})\psi_n(\vec{k}).$$
(4.2.45)

Keep mind, that the Dirac indices are suppressed in all these expressions. Really, ψ_n is a matrix, and \bar{s} is a two matrix. This of course has to do with possible spin orientations of the electron and the anti-particle. Let us use the expression for \bar{s} eq. (4.2.36) and write the Dirac indices out explicitly but suppress the momentum convolution:

$$(\psi_n)_{ab} = \frac{N}{4} \frac{(1 - \gamma_0)_{ea}^{(1)} (1 + \gamma_0)_{bf}^{(2)}}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} i \vec{K}_{ef;gh}(\psi_n)_{gh}.$$
(4.2.46)

Since $(1 - \gamma_0)(1 + \gamma_0) = 0$, it follows from eq. (4.2.46) that

$$(1 + \gamma_0)_{aa'}(\psi_n)_{ab} = 0 \qquad (1 - \gamma_0)_{b'b}(\psi_n)_{ab} = 0 (1 + \gamma_0)^T \psi_n = 0 \qquad \psi_n (1 - \gamma_0)^T = 0.$$
(4.2.47)

There are four orthonormal matrices X^{sm} satisfying these relations, and we choose them in such a way that they are the eigenvectors of the spin operator.

$$X^{sm} = \begin{pmatrix} 0 & \xi^{sm} \\ 0 & 0 \end{pmatrix} \tag{4.2.48}$$

$$\xi^{00} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix} \qquad \xi^{10} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix} \qquad \xi^{11} = \begin{pmatrix} 0 & -1\\ 0 & 0 \end{pmatrix} \qquad \xi^{1,-1} = \begin{pmatrix} 0 & 0\\ 1 & 0 \end{pmatrix}$$

With their orthogonality relation

$$\operatorname{tr}\left[X^{\dagger s'm'}X^{sm}\right] = X^{\dagger s'm'}_{ab}X^{sm}_{ba} = \delta_{ss'}\delta_{mm'}$$

$$(4.2.49)$$

The solution then is a superposition of these matrices:

$$\psi_n = \sum_{sm} X^{sm} \phi_n^{sm}, \qquad (4.2.50)$$

where ϕ_n^{sm} will correspond to the wavefunction of the Schrödinger equation with spin quantum numbers s, m. Expressing ψ in terms of ϕ :

$$\sum_{s''m''} X_{ab}^{s''m''} \phi_n^{s''m''} = \frac{N}{4} \frac{(1 - \gamma_0)_{ea}^{(1)} (1 + \gamma_0)_{bf}^{(2)}}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} i \bar{K}_{ef;gh} \sum_{s'm'} X_{gh}^{s'm'} \phi_n^{s'm'}.$$
(4.2.51)

We would like to single out the equation for ϕ_n^{sm} , to do that use the orthogonality relation for the spin matrices:

$$\sum_{s''m''} X_{ba}^{\dagger sm} X_{ab}^{s''m''} \phi_n^{s''m''} = \frac{N}{4} \frac{(1 - \gamma_0)_{ea}^{(1)} X_{ba}^{\dagger sm} (1 + \gamma_0)_{bf}^{(2)}}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} i\bar{K}_{ef;gh} \sum_{s'm'} X_{gh}^{s'm'} \phi_n^{s'm'}, \qquad (4.2.52)$$

$$\phi_n^{sm} = \frac{N}{4} \frac{\left[(1 - \gamma_0)^{(1)} X^{*sm} (1 + \gamma_0)^{(2)} \right]_{ef}}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} i \bar{K}_{ef;gh} \sum_{s'm'} X_{gh}^{s'm'} \phi_n^{s'm'}, \qquad (4.2.53)$$

$$\phi_n^{sm} = N \frac{1}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} \sum_{s'm'} X_{ef}^{sm} i \bar{K}_{ef;gh} X_{gh}^{s'm'} \phi_n^{s'm'}.$$
(4.2.54)

The trace on the right hand side of this equation represents how different spin states are mixed through the kernel. We define a shorthand:

$$\hat{K}^{sm;s'm'} = X_{ef}^{sm} \bar{K}_{ef;gh} X_{gh}^{s'm'}.$$
(4.2.55)

Finally, let us restore the momentum convolution:

$$\phi_n^{sm} = N \frac{1}{-\frac{\gamma^2}{2m_r} - \frac{\vec{p}^2}{2m_r} + i\epsilon} \sum_{s'm'} \int \frac{d^3k}{(2\pi)^3} i\hat{K}^{sm;s'm'}(P;\vec{p},\vec{q})\phi_n^{s'm'}(\vec{q}).$$
(4.2.56)

It remains to choose a suitable approximation of the kernel, K_0 . Let us choose the Coulomb kernel corrected by a factor of 1/N (keep in mind that $1/N \approx 1$, so K_0 approximates the Coulomb kernel well):

$$K_0 = i \frac{(ie\gamma_0)^{(1)}(ie\gamma_0)^{(2)}}{|\vec{p} - \vec{q}\,|^2} \frac{1}{N} = -ie^2 \frac{\gamma_0^{(1)}\gamma_0^{(2)}}{|\vec{p} - \vec{q}\,|^2} \frac{1}{N}$$
(4.2.57)

$$\hat{K}_{0}^{sm;s'm'} = i \frac{e^2}{|\vec{p} - \vec{q}\,|^2} \frac{1}{N} \delta_{ss'} \delta_{mm'} \tag{4.2.58}$$

As one can see, this choice of kernel leads to the Coulomb-Schrödinger equation:

$$\left(\mathcal{E}_{n}^{0} - \frac{\vec{p}^{2}}{2m_{r}}\right)\phi_{n}^{sm}(\vec{p}) = -\int \frac{d^{3}k}{(2\pi)^{3}} \frac{e^{2}}{|\vec{p} - \vec{q}\,|^{2}}\phi_{n}^{sm}(\vec{q}\,),\tag{4.2.59}$$

where we have identified the binding energy \mathcal{E} :

$$\mathcal{E}_n^0 = -\frac{\gamma^2}{2m_r}.\tag{4.2.60}$$

4.3 Perturbation theory

Let us summarize what we did leading up to this point. We have started with the renormalized Dyson equation with the 2PI irreducible kernel K_R :

$$G_R = S_R + S_R K_R G_R. aga{4.3.1}$$

We have transformed the equation by a choosing a different propagator S_0 , yet keeping the bound states poles unaltered through compensating changes in the kernel K:

$$G = S_0 + S_0 KG, K = K_R + K_R (S_R - S_0) K.$$
(4.3.2)

At this point the equation is still in principle exact, but hardly solvable. We proceed by approximating the kernel K by its dominant part K_0 , to obtain an exactly solvable problem, in this particular case, the Coulomb-Schrödinger equation:

$$G_0 = S_0 + S_0 K_0 G_0. (4.3.3)$$

It remains to relate the exact poles of G, $\{E_n\}$ to the poles of the zeroth order GF G_0 , $\{E_n^0\}$. In order to do that, we should first relate the true GF G to the approximation G_0 through some sort of a perturbation expansion. This can be done by eliminating S_0 form eq. (4.3.2) and eq. (4.3.3). First notice that eq. (4.3.3) maybe rewritten by expanding the series on the right side and resuming it in another way:

$$G_0 = S_0 + G_0 K_0 S_0, (4.3.4)$$

$$S_0 = (1 + G_0 K_0)^{-1} G_0. (4.3.5)$$

Using the transformed version of eq. (4.3.2):

$$G = (1 - S_0 K)^{-1} S_0.$$

= $(1 - S_0 K)^{-1} (1 + G_0 K_0)^{-1} G_0$
= $[(1 + G_0 K_0) (1 - S_0 K)]^{-1} G_0$
= $[1 + G_0 K_0 - S_0 K - G_0 K_0 S_0 K]^{-1} G_0$
= $(1 - G_0 \delta K)^{-1} G_0.$

Expanding in powers of δK :

$$G = G_0 + G_0 \delta K G_0 + G_0 \delta K G_0 \delta K G_0 + \mathcal{O}(\delta K^3).$$

$$(4.3.6)$$

We can use this result to relate E_n to E_n^0 . Take two arbitrary matrices A and B and note the following result:

$$E_n - E_n^0 = \frac{\oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A G(E) B}{\oint_{C_n} \frac{dE}{2\pi i} A G(E) B},$$
(4.3.7)

where C_n is the contour in the complex E plane that only contains one pole of G at E_n and one pole of G_0 at E_n^0 (as usual the sum over Dirac indices and the momentum convolution is suppressed). We wish to keep corrections of order $(\delta K)^2$, which means the numerator has to be expanded to order $(\delta K)^2$, but the denominator only needs to be expanded up to order δK :

$$E_n - E_n^0 = \frac{\oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A(G_0 + G_0 \delta K G_0 + G_0 \delta K G_0 \delta K G_0) B}{\oint_{C_n} \frac{dE}{2\pi i} A(G_0 + G_0 \delta K G_0) B}.$$
(4.3.8)

Notice the first term in the numerator is analytic, so it does not contribute to the contour integral.

$$E_n - E_n^0 = \frac{\oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A (G_0 \delta K G_0 + G_0 \delta K G_0 \delta K G_0) B}{\oint_{C_n} \frac{dE}{2\pi i} A (G_0 + G_0 \delta K G_0) B}.$$
 (4.3.9)

Now let us consider the second term in the numerator:

2nd term =
$$\oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A G_0 \delta K G_0 B$$

=
$$\oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) \delta K \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) B$$

=
$$- [A \Psi_n^0] [\bar{\Psi}_n^0 \delta K \Psi_n^0] [\bar{\Psi}_n^0 B],$$

where we have used the brackets to make several traces present in the expression more evident. Each energy dependent term is to be evaluated at E_n^0 after integration, for now we suppress the evaluation. Now, consider the third term:

$$3 \text{rd term} = \oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A G_0 \delta K G_0 \delta K G_0 B$$

$$= \oint_{C_n} \frac{dE}{2\pi i} (E - E_n^0) A \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) \delta K \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) \delta K \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) \delta K \left(i \frac{\Psi_n^0 \bar{\Psi}_n^0}{E - E_n^0} + \tilde{G}_0 \right) B$$

$$= - \left[A \Psi_n^0 \right] \left[\bar{\Psi}_n^0 \delta K \Psi_n^0 \right] \left[\bar{\Psi}_n^0 \delta K \tilde{G}_0 B \right] - \left[A \Psi_n^0 \right] \left[\bar{\Psi}_n^0 \delta K \tilde{G}_0 \delta K \Psi_n^0 \right] \left[\bar{\Psi}_n^0 \delta K \Psi_n^0 \right] \left[\bar{\Psi}_n^0$$

Now let us expand the denominator:

-

$$denom. = \frac{1}{\oint_{C_n} \frac{dE}{2\pi i} A(G_0 + G_0 \delta K G_0) B}}$$
$$= \frac{1}{\oint_{C_n} \frac{dE}{2\pi i} A G_0 B} \left(1 - \frac{\oint_{C_n} \frac{dE}{2\pi i} A G_0 \delta K G_0 B}{\oint_{C_n} \frac{dE}{2\pi i} A G_0 B} \right)$$
$$= \frac{1}{i [A\Psi_n^0] [\bar{\Psi}_n^0 B]} \left(1 - \frac{i [A\Psi_n^0] [\bar{\Psi}_n^0 \delta K \tilde{G}_0 B] + i [A \tilde{G}_0 \delta K \Psi_n^0] [\bar{\Psi}_n^0 B] - \frac{d}{dE} [A \Psi_n^0] [\bar{\Psi}_n^0 \delta K \Psi_n^0] [\bar{\Psi}_n^0 B]}{i [A \Psi_n^0] [\bar{\Psi}_n^0 B]} \right)$$

Combining everything and only keeping terms up to $(\delta K)^2$, we get

$$E_n - E_n^0 = i \left[\bar{\Psi}_n^0 \delta K \Psi_n^0 \right] \left(1 + i \left[\bar{\Psi}_n^0 \frac{d}{dE} \delta K \Psi_n^0 \right] \right) \Big|_{E=E_n^0} + i \left[\bar{\Psi}_n^0 \delta K \widetilde{G}_0 \delta K \Psi_n^0 \right] \Big|_{E=E_n^0}$$

$$(4.3.10)$$

Chapter 5

Ground state HFS in positronium

5.1 Polarization vectors

In this section we will apply the method described above to calculate the hyperfine splitting in the ground state of positronium, in other words the mass difference between orthopositronium (o-Ps) and para-positronium (p-Ps). Recall that p-Ps is the triplet state with aligned spins, such that the total spin is s = 1, and the projection can be m = -1, 0, 1. Whereas o-Ps is the singlet state with s = 0, m = 0. As we have already mentioned the spin matrices corresponding to these states are:

$$X^{sm} = \begin{pmatrix} 0 & \xi^{sm} \\ 0 & 0 \end{pmatrix} \tag{5.1.1}$$

$$\underbrace{\xi^{00} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0\\ 0 & 1 \end{pmatrix}}_{\text{the singlet}} \qquad \underbrace{\xi^{10} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix}}_{\text{the triplet}} \qquad \underbrace{\xi^{11} = \begin{pmatrix} 0 & -1\\ 0 & 0 \end{pmatrix}}_{\text{the triplet}} \qquad \underbrace{\xi^{1,-1} = \begin{pmatrix} 0 & 0\\ 1 & 0 \end{pmatrix}}_{\text{the triplet}} \quad (5.1.2)$$

For future convenience, let us express these states in terms of Pauli matrices and polarization vectors:

$$\xi^{00} = \frac{1}{\sqrt{2}} \mathbb{1}$$

$$\xi^{1m} = \frac{1}{\sqrt{2}} \vec{\epsilon}_{(m)} \cdot \vec{\sigma} \quad \begin{cases} \vec{\epsilon}_{(0)} = (0, 0, 1) \\ \vec{\epsilon}_{(\pm)} = \frac{-1}{\sqrt{2}} (\pm 1, i, 0) \end{cases}$$

$$\vec{\epsilon}_{(m)} \cdot \vec{\epsilon}_{(n)}^{*} = \delta_{mn}.$$
(5.1.3)

Notice that the subscript (m) on $\vec{\epsilon}_{(m)}$ is not to be confused with a component of the vector, but rather it spans a family of different vectors. However, whenever we write a subscript without parentheses, such as $\epsilon_{(m)i}$, we mean the *i*'th component of the vector $\vec{\epsilon}_{(m)}$. Since in this calculation different polarizations are never mixed in the same equation, we will generally suppress the subscript (m) until the very end of the calculation, where we restore it.

5.2 Ground state wavefunction

Solution of the Coulomb-Schrödinger equation in quantum mechanics are characterized by three quantum numbers: the principal quantum number n, the angular momentum quantum number ℓ , and the magnetic quantum number m. Unless other interactions are added perturbatively, the energy of different states only depends on the principal quantum number and is completely degenerate in ℓ and m:

$$\mathcal{E}_n^0 = -\frac{m_r \alpha^2}{2n^2}, \quad n = 1, 2, 3...$$
(5.2.1)

The way one generally proceeds in quantum mechanics, is to add small perturbations to the original Hamiltonian, and calculate the resulting shifts in energy. For example, if one considers spin-orbit coupling (LS-coupling) the energy corrections to states with different angular quantum number ℓ will be different, breaking the degeneracy in ℓ . This splitting of states with different ℓ is known as the fine splitting. Notice that in the ground state n = 1, the only allowed value for the angular momentum number is $\ell = 0$, and fine splitting does not appear.

What we will be mainly concerned with is the hyperfine splitting (hfs), which appears because of the spin-spin coupling (SS-coupling). In this section we will calculate the hyperfine splitting in the ground state for positronium using the quasipotential approach to the BSE in QED. To do this, we need the ground state wavefunction and its Fourier transform:

$$\phi(\vec{x}\,) = \sqrt{\frac{\gamma^3}{\pi}} e^{-\gamma r} \qquad \phi(\vec{p}\,) = \mathcal{F}\{\phi(\vec{p}\,)\} = \sqrt{\frac{\gamma^3}{\pi}} \frac{8\pi\gamma}{(\vec{p}\,^2 + \gamma^2)^2} \tag{5.2.2}$$

We can also infer from eq. (4.2.60) and eq. (5.2.1) that

$$\gamma = m_r \alpha \tag{5.2.3}$$

in the ground state. We can see from the wavefunction in position space, $1/\gamma$ is the Bohr radius. If we now look at the momentum space wavefunction, we can see that γ acts as somewhat of a natural energy cut-off, suppressing the wavefunction for high momenta. This is crucial for the perturbation theory set up in section 4.3 to work. To better understand why, consider the correction to the kernel K_0

$$\delta K = K_C (S_R - S_0) K_C, \qquad (5.2.4)$$

and the resulting contribution to the energy shift:

$$\delta E = \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \phi(\vec{p}) i K_C (S_R - S_0) K_C \phi(\vec{q}).$$
(5.2.5)

By construction, S_0 approximates S_R well in the non-relativistic regime, such that $(S_R - S_0)$ is small. So in the non-relativistic regime, where the bulk of the wavefunction is concentrated, the integral is suppressed by the small difference in propagators. In the relativistic regime, where S_R is not necessarily close to S_0 , the integral is suppressed by the wavefunction itself. Understanding this structure of scales of the problem plays a key role in estimating contributions to the energy from different kernel corrections since simply counting the number of diagram vertices does not work.

5.3 The transverse photon and annihilation

Let us move on to the actual calculation of the hfs. What correction to the kernel produces it? Since we know the hfs exists because of the spin-spin interaction, we are looking for a spin dependent kernel. Consider the simplest such kernel, transverse photon exchange:



Figure 5.3.1: Transverse photon exchange correction.

For this kernel, we have:

$$\bar{K}_{ef;gh}(P;\vec{p},\vec{q}\,) = \left(ie\gamma_i\right)_{ge} \left(ie\gamma_j\right)_{fh} \Delta^{ij}(\vec{p}-\vec{q}\,) \tag{5.3.1}$$

The simplest correction to the energy from this kernel is

$$\delta E_T^{sm} = i \Big[\bar{\psi} \bar{K} \psi \Big] = \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \phi(\vec{p}) X_{ef}^{sm} i \bar{K}_{ef;gh}(P;\vec{p},\vec{q}) X_{gh}^{sm} \phi(\vec{q}) = \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \phi(\vec{p}) \operatorname{Tr} \Big[(i e \gamma_i) X^{sm} (i e \gamma_j) X^{\dagger sm} \Big] \phi(\vec{q})$$
(5.3.2)

At this point we should mention a very important property of the BSE wavefunction ψ . From eq. (4.2.46) it follows that large and small projectors don't alter ψ provided they are acted from the correct side:

$$\psi = P_{-}\psi P_{+}, \qquad \psi^{\dagger} = P_{+}\psi^{\dagger}P_{-}$$
 (5.3.3)

where

$$P_{+} = \frac{1}{2}(1 + \gamma_{0}) \qquad P_{-} = \frac{1}{2}(1 - \gamma_{0})$$

$$P_{+}P_{+} = P_{+} \qquad P_{+}P_{-} = P_{-}P_{+} = 0 \qquad P_{-}P_{-} = P_{-}$$

$$P_{+}\gamma_{i}P_{+} = 0 = P_{-}\gamma_{i}P_{-}$$
(5.3.4)

It follows that

$$\delta E_T^{sm} = \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \phi(\vec{p}) \operatorname{Tr} \left[P_-(ie\gamma_i) P_- X^{sm} P_+(ie\gamma_j) P_+ X^{\dagger sm} \right] \phi(\vec{p}) = 0.$$
(5.3.5)

The contribution from transverse photon exchange vanishes. The next thing we can check is the annihilation diagram, for which the corresponding kernel is



Figure 5.3.2: The annihilation correction.

$$\bar{K}_{ef;gh} = \left(ie\gamma_{\mu}\right)_{fe} \left(ie\gamma_{\nu}\right)_{gh} \Delta^{\mu\nu}(E,\vec{0}).$$
(5.3.6)

The energy correction resulting from this kernel is:

$$\delta E_{a}^{sm} = i \Big[\bar{\psi} \bar{K} \psi \Big] = \int \frac{d^{3}p}{(2\pi)^{3}} \frac{d^{3}q}{(2\pi)^{3}} \phi(\vec{p}) X_{ef}^{sm} i \bar{K}_{ef;gh}(P;\vec{p},\vec{q}) X_{gh}^{sm} \phi(\vec{q}) = -ie^{2} \int \frac{d^{3}p}{(2\pi)^{3}} \frac{d^{3}q}{(2\pi)^{3}} \phi(\vec{p}) \operatorname{Tr} \left[\gamma_{\mu} X^{sm} \right] \operatorname{Tr} \left[X^{\dagger sm} \gamma_{\nu} \right] \Delta^{\mu\nu}(E,\vec{0}) \phi(\vec{q}).$$
(5.3.7)

Let us first consider temporal traces $\mu, \nu = 0$, using the property of the wavefunction described in eq. (5.3.3):

$$\operatorname{Tr}\left[\gamma_{0}P_{-}X^{sm}P_{+}\right]\operatorname{Tr}\left[P_{+}X^{\dagger sm}P_{-}\gamma_{0}\right]$$
$$=\operatorname{Tr}\left[P_{+}P_{-}X^{sm}\right]\operatorname{Tr}\left[P_{-}P_{+}X^{\dagger sm}\right]$$
$$= 0.$$
(5.3.8)

One can see that the temporal part does not contribute, so we should consider the spatial part $\mu, \nu = i, j$:

$$\operatorname{Tr}\left[\gamma_{i}X^{sm}\right]\operatorname{Tr}\left[X^{\dagger sm}\gamma_{j}\right]$$

$$=\operatorname{Tr}\left[\begin{pmatrix}0 & \sigma_{i}\\-\sigma_{i} & 0\end{pmatrix}\begin{pmatrix}0 & \xi^{sm}\\0 & 0\end{pmatrix}\right]\operatorname{Tr}\left[\begin{pmatrix}0 & \sigma_{j}\\-\sigma_{j} & 0\end{pmatrix}\begin{pmatrix}0 & 0\\\xi^{\dagger sm} & 0\end{pmatrix}\right]$$

$$=-\operatorname{Tr}\left[\sigma_{i}\xi^{sm}\right]\operatorname{Tr}\left[\sigma_{j}\xi^{\dagger sm}\right].$$
(5.3.9)

We can see that this part can produce hfs, because it might contribute different energy shifts to the singlet and the triplet. Let us consider the contribution to the singlet state, $\xi^{00} = \frac{1}{\sqrt{2}} \mathbb{1}:$

$$\operatorname{Tr}[\gamma_{i}X^{00}]\operatorname{Tr}[X^{\dagger00}\gamma_{j}] = -\operatorname{Tr}[\sigma_{i}\xi^{00}]\operatorname{Tr}[\sigma_{j}\xi^{\dagger00}] = -\frac{1}{2}\operatorname{Tr}[\sigma_{i}]\operatorname{Tr}[\sigma_{j}] \qquad (5.3.10) = 0,$$

so this kernel does not contribute any energy to the singlet:

$$\delta E_a^{00} = 0. \tag{5.3.11}$$

Now, compute the contribution to the triplet, $\xi^{1m} = \frac{1}{\sqrt{2}} \vec{\epsilon}_{(m)} \cdot \vec{\sigma}$ (we suppress the index (m) on the polarization vector):

$$\operatorname{Tr}[\gamma_{i}X^{1m}]\operatorname{Tr}[X^{\dagger 1m}\gamma_{j}] = -\operatorname{Tr}[\sigma_{i}\xi^{1m}]\operatorname{Tr}[\sigma_{j}\xi^{\dagger 1m}] = -\frac{1}{2}\epsilon_{k}\epsilon_{n}^{*}\operatorname{Tr}[\sigma_{i}\sigma_{k}]\operatorname{Tr}[\sigma_{j}\sigma_{n}]$$

$$= 2\epsilon_{k}\epsilon_{n}^{*}\delta_{ik}\delta_{jn}$$

$$= 2\epsilon_{i}\epsilon_{j}^{*}.$$
(5.3.12)

Having computed the trace, we can compute the shift in energy:

$$\delta E_a^{1m} = 2ie^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \phi(\vec{p}\,) \epsilon_i \epsilon_j^* \Delta^{ij}(E,\vec{0}) \phi(\vec{q}\,), \tag{5.3.13}$$

where we can now explicitly state the transverse photon propagator at zero momentum:

$$\delta E_a^{1m} = 2ie^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \phi(\vec{p}\,) \epsilon_i \epsilon_j^* \frac{i}{E^2} \delta^{ij} \phi(\vec{q}\,) = \frac{2e^2}{E^2} \left(\vec{\epsilon}_{(m)} \cdot \vec{\epsilon}_{(m)}^*\right) \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \phi(\vec{p}\,) \phi(\vec{q}\,)$$
(5.3.14)
$$= \frac{2e^2}{E^2} \phi(\vec{x}=0)^2$$

As one can see, the energy shift only depends on the norm of the polarization vector, so that every state in the triplet gets the same contribution. Since we are only interested in the leading order contribution, we set $E = 2\sqrt{m_e^2 - \gamma^2} \approx 2m_e$, though in principle one can see that even this kernel contributes to all orders in α , because of the γ dependence in the denominator. This of course has to be taken into account when one computes the higher order corrections. Substituting the value of the wavefunction, we get:

$$\delta E_a^{1m} - \delta E_a^{00} = \frac{m_e \alpha^4}{4}.$$
(5.3.15)

This is the simplest contribution to the hfs in our framework. However, notice that this is already impossible to obtain in the context of quantum mechanics, since there is no way to account for annihilation.

5.4 Crossed cancelations

The next correction to consider in δK is the crossed photon exchange on fig. 5.4.1. Recall that the simple two photon exchange is **not** in $\delta K = K_R - K_0 + K_R(S_R - S_0)K_R + \dots$, since it is a reducible diagram.



Figure 5.4.1: The crossed photon contribution from δK .



Figure 5.4.2: The double exchange is **not** in δK .

However, there is indeed a diagram in δK that very much resembles the double exchange, and it is contained in the propagator correction part $K_R(S_R - S_0)K_R$. If we simply take the single exchange part of K_R on both sides, and denote the difference of propagators with a blob on the diagram, the contribution will look like fig. 5.4.3:



Figure 5.4.3: A contribution from $K_R(S_R - S_0)K_R$.

As we will demonstrate here, *if these diagrams are treated together they need not be computed, as they do not contribute to the hfs.* We find this is easier to see if the transverse and Coulomb photons are treated separately (although the mixed terms are also present of course). Let us start by considering the contributions with two transverse photons.

5.4.1 Two transverse photons

Within this section, we call the crossed transverse contribution K^c and the double transverse photon exchange K^d . The sum of the two is denoted K^{TT} .



Figure 5.4.4: The contribution with two transverse photons.

$$K^{c}_{ef;gh} = \int \frac{d^{4}k}{(2\pi)^{4}} \left[(ie\gamma_{\ell})\Delta(E'\delta^{\mu}_{0} + k^{\mu})(ie\gamma_{i}) \right]_{ge} \left[(ie\gamma_{m})\Delta(-E'\delta^{\mu}_{0} + k^{\mu})(ie\gamma_{j}) \right]_{fh} \qquad (5.4.1)$$
$$\times \Delta^{ij}(p-k)\Delta^{\ell m}(k-q)$$

To eventually compute the energy contribution, we first need to compute the trace

$$\hat{K}^c = X_{ef} K^c_{ef;gh} X_{gh}.$$
(5.4.2)

$$\hat{K}^{c} = \int \frac{d^{4}k}{(2\pi)^{4}} \operatorname{Tr}\left[(ie\gamma_{\ell})\Delta(E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{i})X(ie\gamma_{m})\Delta(-E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{j})X^{\dagger}\right] \times \Delta^{ij}(p-k)\Delta^{\ell m}(k-q)$$
(5.4.3)

We can simplify this by doing two things: split electron and positron propagators into small and large projectors and use eq. (5.3.3). Having done this, the propagators are

$$\Delta(E'\delta_0^{\mu} + k^{\mu}) = -i \frac{-E'\gamma_0 - k^0\gamma_0 - k^i\gamma_i + m_e}{-(E' + k^0)^2 + \vec{k}\,^2 + m_e^2 - i\epsilon}$$

= $\frac{P_-(E' + k^0 + m_e) - P_+(E' + k^0 - m_e) - \vec{k} \cdot \vec{\gamma}}{D(k)},$ (5.4.4)

$$\Delta(-E'\delta_0^{\mu} + k^{\mu}) = -i \frac{E'\gamma_0 - k^0\gamma_0 - k^i\gamma_i + m_e}{-(-E' + k^0)^2 + \vec{k}\,^2 + m_e^2 - i\epsilon}$$

= $\frac{P_-(-E' + k^0 + m_e) - P_+(-E' + k^0 - m_e) - \vec{k} \cdot \vec{\gamma}}{D(-k)},$ (5.4.5)

$$D(k) = i \left[-(E'+k^0)^2 + \vec{k}^2 + m_e^2 - i\epsilon \right]$$
(5.4.6)

where P_+, P_- are the large and small projectors. With this decomposition and eq. (5.3.3) in mind, we can rewrite the trace in eq. (5.4.3) as

$$\frac{1}{D(k)D(-k)} \operatorname{Tr} \left[P_{-}(ie\gamma_{\ell}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{i}) P_{-} X \right] \times P_{+}(ie\gamma_{m}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{j}) P_{+} X^{\dagger},$$
(5.4.7)

where we have not stated the coefficients of projectors for now, and we have used the cyclicity of the trace to move the P_{-} from the very end to the very beginning. Now, we can use the fact that an expression with an odd number of spatial gamma matrices between two same projectors (such as $P_{-}(ie\gamma_{\ell})P_{-}$) vanishes, to simplify the trace

$$\frac{1}{D(k)D(-k)} \operatorname{Tr} \left[P_{-}(ie\gamma_{\ell}) \left[-P_{+}(E'+k^{0}-m_{e}) \right] (ie\gamma_{i}) P_{-}X \right] \times P_{+}(ie\gamma_{m}) \left[P_{-}(-E'+k^{0}+m_{e}) \right] (ie\gamma_{j}) P_{+}X^{\dagger},$$
(5.4.8)

where we have restated the coefficients of P_+ and P_- . We can now commute the inner projectors toward the outer ones such as $P_+(ie\gamma_m)P_- = P_+P_+(ie\gamma_m) = (ie\gamma_m)$, and reabsorb the projectors into the wavefunctions to get

$$-\frac{(E'+k^0-m_e)(-E'+k^0+m_e)}{D(k)D(-k)}\operatorname{Tr}\left[(ie\gamma_\ell)(ie\gamma_i)X(ie\gamma_m)(ie\gamma_j)X^{\dagger}\right].$$
(5.4.9)

Let us state what \hat{K}^c looks like after these simplifications, and move on to \hat{K}^d for now.

$$\hat{K}^{c} = -\int \frac{d^{4}k}{(2\pi)^{4}} \frac{(E'+k^{0}-m_{e})(-E'+k^{0}+m_{e})}{D(k)D(-k)} \Delta^{ij}(p-k)\Delta^{\ell m}(k-q) \times \operatorname{Tr}\left[(ie\gamma_{\ell})(ie\gamma_{i})X(ie\gamma_{m})(ie\gamma_{j})X^{\dagger}\right]$$
(5.4.10)

As we have stated before, the \hat{K}^d contribution is of the form $K^T(S_R - S_0)K^T$, where K^T is transverse photon exchange. We will first compute the second part of this expression, that is $(-K^T S_0 K^T)$. Recall that the matrix part of S_0 is simply P_- for the electron and P_+ for the positron. So the trace part of this contribution will be

$$\operatorname{Tr}\left[(ie\gamma_{\ell})P_{-}(ie\gamma_{i})X(ie\gamma_{j})P_{+}(ie\gamma_{m})X^{\dagger}\right] = \operatorname{Tr}\left[P_{-}(ie\gamma_{\ell})P_{-}(ie\gamma_{i})P_{-}XP_{+}(ie\gamma_{j})P_{+}(ie\gamma_{m})P_{+}X^{\dagger}\right]$$
(5.4.11)
= 0,

such that the contribution vanishes. This means we are left with the $K^T S_R K^T$ bit of it, which is simply eq. (5.4.3) with the vertex factors $(ie\gamma_m)$ and $(ie\gamma_j)$ exchanged:

$$\hat{K}^{d} = \int \frac{d^{4}k}{(2\pi)^{4}} \operatorname{Tr}\left[(ie\gamma_{\ell})\Delta(E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{i})X(ie\gamma_{j})\Delta(-E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{m})X^{\dagger}\right] \times \Delta^{ij}(p-k)\Delta^{\ell m}(k-q).$$
(5.4.12)

Since all of the arguments we used to simplify eq. (5.4.3) also hold for the trace in \hat{K}^d , the simplified version of \hat{K}^d is simply eq. (5.4.10) with $(ie\gamma_m)$ and $(ie\gamma_j)$ exchanged

$$\hat{K}^{d} = -\int \frac{d^{4}k}{(2\pi)^{4}} \frac{(E'+k^{0}-m_{e})(-E'+k^{0}+m_{e})}{D(k)D(-k)} \Delta^{ij}(p-k)\Delta^{\ell m}(k-q) \times \operatorname{Tr}\left[(ie\gamma_{\ell})(ie\gamma_{i})X(ie\gamma_{j})(ie\gamma_{m})X^{\dagger}\right].$$
(5.4.13)

Notice that when we add the two contributions \hat{K}^c and \hat{K}^d , we can use the anticommutation relations for the Dirac matrices, $\{\gamma_j, \gamma_m\} = -2\delta_{jm}$. Taking this into account,

$$\hat{K}^{c} + \hat{K}^{d} = -2e^{2} \int \frac{d^{4}k}{(2\pi)^{4}} \frac{(E' + k^{0} - m_{e})(-E' + k^{0} + m_{e})}{D(k)D(-k)} \Delta^{ij}(p-k)\Delta^{\ell j}(k-q) \times \operatorname{Tr}\left[(ie\gamma_{\ell})(ie\gamma_{i})XX^{\dagger}\right].$$
(5.4.14)

This is quite a lot simpler than what we had in the beginning, but still it is not obvious why these diagrams do not contribute to the hfs. In order to understand that, we need to integrate these contributions with the wavefunctions in order to find the energy contribution:

$$\delta E = 2e^2 \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{(E' + k^0 - m_e)(-E' + k^0 + m_e)}{D(k)D(-k)}$$

$$\times \Delta^{ij}(p-k)\Delta^{\ell j}(k-q)\phi(\vec{p})\phi(\vec{q}) \operatorname{Tr}\left[(ie\gamma_\ell)(ie\gamma_i)XX^{\dagger}\right].$$
(5.4.15)

Now, let us rename the dummy momenta $\vec{p} \leftrightarrow \vec{q}$, and the dummy indices $\ell \leftrightarrow i$:

$$\delta E = 2e^2 \int \frac{d^3 p}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3} \frac{d^4 k}{(2\pi)^4} \frac{(E' + k^0 - m_e)(-E' + k^0 + m_e)}{D(k)D(-k)}$$

$$\times \Delta^{\ell j} (q - k) \Delta^{ij} (k - p) \phi(\vec{q}) \phi(\vec{p}) \operatorname{Tr} \left[(ie\gamma_i)(ie\gamma_\ell) X X^{\dagger} \right].$$
(5.4.16)

Now, if we take into account that the transverse photon is even in momentum $\Delta^{ij}(p) = \Delta^{ij}(-p)$, we can see that after this renaming, the only thing in eq. (5.4.15) that is changed is the position of the gamma matrices in the trace

$$\delta E = 2e^2 \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{d^4k}{(2\pi)^4} \frac{(E'+k^0-m_e)(-E'+k^0+m_e)}{D(k)D(-k)}$$

$$\times \Delta^{ij}(p-k)\Delta^{\ell j}(k-q)\phi(\vec{p})\phi(\vec{q}) \operatorname{Tr}\left[(ie\gamma_i)(ie\gamma_\ell)XX^{\dagger}\right].$$
(5.4.17)

If we now add eq. (5.4.15) to eq. (5.4.17), divide by 2, and use the anticommutation relation again, we obtain

$$\delta E = 2e^4 \int \frac{d^3p}{(2\pi)^3} \frac{d^3q}{(2\pi)^3} \frac{d^4k}{(2\pi)^4} \frac{(E'+k^0-m_e)(-E'+k^0+m_e)}{D(k)D(-k)}$$

$$\times \Delta^{ij}(p-k)\Delta^{ij}(k-q)\phi(\vec{p})\phi(\vec{q}) \operatorname{Tr} \left[XX^{\dagger}\right].$$
(5.4.18)

Finally, we can see that indeed, this sum cannot contribute to the hfs, since the trace $\text{Tr}[XX^{\dagger}] = 1$, regardless of whether X is the singlet or one of the triplets, so that both the singlet and the triplet get the same energy contribution, and there is no splitting produced.

5.4.2 A transverse photon and a Coulomb photon

The next thing to consider is the same contribution with one of the photons being a Coulomb photon:



Figure 5.4.5: The contribution with a transverse photon and a Coulomb photon.

Within this section, we will again call the crossed contribution K^c , and the double contribution K^d . Let us start with the crossed diagram:

$$\hat{K}^{c} = \int \frac{d^{4}k}{(2\pi)^{4}} \operatorname{Tr}\left[(ie\gamma_{0})\Delta(E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{i})X(ie\gamma_{0})\Delta(-E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{j})X^{\dagger}\right] \times \Delta^{ij}(p-k)\Delta^{00}(k-q)$$
(5.4.19)

We will proceed the same way we did before, by splitting the propagators into projectors, and rewriting the wavefunctions. Then the trace in this expression is

$$\frac{1}{D(k)D(-k)} \operatorname{Tr} \left[P_{-}(ie\gamma_{0}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{i}) P_{-} X \right] \times P_{+}(ie\gamma_{0}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{j}) P_{+} X^{\dagger} , \qquad (5.4.20)$$

and by using the properties of projectors in eq. (5.3.4), we obtain:

$$= \frac{1}{D(k)D(-k)} \operatorname{Tr} \left[P_{-}(ie\gamma_{0}) \left[-\vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{i}) P_{-} X \\ \times P_{+}(ie\gamma_{0}) \left[-\vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{j}) P_{+} X^{\dagger} \right]$$

$$= \frac{e^{2}}{D(k)D(-k)} \operatorname{Tr} \left[P_{-} \left[-\vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{i}) P_{-} X \\ \times P_{+} \left[-\vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{j}) P_{+} X^{\dagger} \right]$$

$$= \frac{e^{2}}{D(k)D(-k)} \operatorname{Tr} \left[\vec{k} \cdot \vec{\gamma} (ie\gamma_{i}) X \ \vec{k} \cdot \vec{\gamma} (ie\gamma_{j}) X^{\dagger} \right]$$
(5.4.21)

With this, eq. (5.4.19) becomes

$$\hat{K}^{c} = \int \frac{d^{4}k}{(2\pi)^{4}} \frac{e^{2}}{D(k)D(-k)} \operatorname{Tr}\left[\vec{k} \cdot \vec{\gamma}(ie\gamma_{i})X \ \vec{k} \cdot \vec{\gamma}(ie\gamma_{j})X^{\dagger}\right] \times \Delta^{ij}(p-k)\Delta^{00}(k-q).$$
(5.4.22)

Following the logic of the previous section, we leave \hat{K}^c for now, and turn to the double photon diagram. Again, we consider two different contributions from this diagram separately. Consider the $-K^T S_0 K^C$ part:

$$\bar{\Psi}K^T S_0 K^C \Psi = N \bar{\Psi} K^T \Psi = 0, \qquad (5.4.23)$$

where we have use the Schrödinger equation $S_0 K_0 \Psi = \Psi$, and the result for the transverse photon.

Now, let us focus on the $K^T S_R K^C$ part.

$$\hat{K}^{d} = \int \frac{d^{4}k}{(2\pi)^{4}} \operatorname{Tr}\left[(ie\gamma_{0})\Delta(E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{i})X(ie\gamma_{j})\Delta(-E'\delta_{0}^{\mu} + k^{\mu})(ie\gamma_{0})X^{\dagger}\right] \times \Delta^{ij}(p-k)\Delta^{00}(k-q)$$
(5.4.24)

Consider the trace

$$\frac{1}{D(k)D(-k)} \operatorname{Tr} \left[P_{-}(ie\gamma_{0}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{i}) P_{-} X \right]$$

$$\times P_{+}(ie\gamma_{j}) \left[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_{0}) P_{+} X^{\dagger} \qquad (5.4.25)$$

$$= \frac{e^{2}}{D(k)D(-k)} \operatorname{Tr} \left[\vec{k} \cdot \vec{\gamma} \ (ie\gamma_{i}) X (ie\gamma_{j}) \vec{k} \cdot \vec{\gamma} \ X^{\dagger} \right],$$

in a manner similar to eq. (5.4.21). With this simplification

$$\hat{K}^{d} = \int \frac{d^{4}k}{(2\pi)^{4}} \frac{e^{2}}{D(k)D(-k)} \operatorname{Tr}\left[\vec{k} \cdot \vec{\gamma} \ (ie\gamma_{i})X(ie\gamma_{j})\vec{k} \cdot \vec{\gamma} \ X^{\dagger}\right]$$

$$\times \Delta^{ij}(p-k)\Delta^{00}(k-q).$$
(5.4.26)

As one can see, the only difference between eq. (5.4.22) and eq. (5.4.26) are the positions of the gamma matrices in th trace. This allows us to simply use the anticommutation relations when adding the two contributions to obtain

$$\hat{K}^{c} + \hat{K}^{d} = \int \frac{d^{4}k}{(2\pi)^{4}} \frac{ie^{3}k^{m}}{D(k)D(-k)} \operatorname{Tr}\left[\vec{k}\cdot\vec{\gamma}\ (ie\gamma_{i})X\{\gamma_{j},\gamma_{m}\}\ X^{\dagger}\right]$$

$$\times \Delta^{ij}(p-k)\Delta^{00}(k-q)$$

$$= \int \frac{d^{4}k}{(2\pi)^{4}} \frac{-2ie^{3}k^{j}}{D(k)D(-k)} \operatorname{Tr}\left[\vec{k}\cdot\vec{\gamma}\ (ie\gamma_{i})XX^{\dagger}\right]$$

$$\times \Delta^{ij}(p-k)\Delta^{00}(k-q).$$
(5.4.27)

Of course, we still have to add the diagrams with the transverse and the Coulomb photon exchanged:

The kernels corresponding to these diagrams can be obtained from eq. (5.4.19) and eq. (5.4.24) by exchanging the appropriate vertex factors and photon propagators:

$$\hat{K}^{c'} = \int \frac{d^4k}{(2\pi)^4} \operatorname{Tr}\left[(ie\gamma_i)\Delta(E'\delta_0^{\mu} + k^{\mu})(ie\gamma_0)X(ie\gamma_j)\Delta(-E'\delta_0^{\mu} + k^{\mu})(ie\gamma_0)X^{\dagger}\right] \times \Delta^{ij}(k-q)\Delta^{00}(p-k)$$

$$\hat{K}^{d'} = \int \frac{d^4k}{(2\pi)^4} \operatorname{Tr}\left[(ie\gamma_i)\Delta(E'\delta_0^{\mu} + k^{\mu})(ie\gamma_0)X(ie\gamma_0)\Delta(-E'\delta_0^{\mu} + k^{\mu})(ie\gamma_j)X^{\dagger}\right] \times \Delta^{ij}(k-q)\Delta^{00}(p-k)$$
(5.4.29)



Figure 5.4.6: The other contribution with a transverse photon and a Coulomb photon.

The traces in these contributions simplify in almost exactly the same manner as previously, so here we just state the result

$$\hat{K}^{c'} = \int \frac{d^4k}{(2\pi)^4} \frac{e^2}{D(k)D(-k)} \operatorname{Tr}\left[(ie\gamma_i)\vec{k}\cdot\vec{\gamma} \ X(ie\gamma_j)\vec{k}\cdot\vec{\gamma} \ X^{\dagger}\right] \times \Delta^{ij}(k-q)\Delta^{00}(p-k)$$
(5.4.30)

$$\hat{K}^{d'} = \int \frac{d^4k}{(2\pi)^4} \frac{e^2}{D(k)D(-k)} \operatorname{Tr}\left[(ie\gamma_i)\vec{k}\cdot\vec{\gamma}\ X\ \vec{k}\cdot\vec{\gamma}\ (ie\gamma_j)X^{\dagger}\right]
\times \Delta^{ij}(k-q)\Delta^{00}(p-k).$$

$$\hat{K}^{c'} + \hat{K}^{d'} = \int \frac{d^4k}{(2\pi)^4} \frac{ie^3k^m}{D(k)D(-k)} \operatorname{Tr}\left[(ie\gamma_i)\vec{k}\cdot\vec{\gamma}\ X\{\gamma_j,\gamma_m\}\ X^{\dagger}\right]
\times \Delta^{ij}(k-q)\Delta^{00}(p-k)
= \int \frac{d^4k}{(2\pi)^4} \frac{-2ie^3k^j}{D(k)D(-k)} \operatorname{Tr}\left[(ie\gamma_i)\vec{k}\cdot\vec{\gamma}\ XX^{\dagger}\right]
\times \Delta^{ij}(k-q)\Delta^{00}(p-k).$$
(5.4.32)

At this point we can see that the structures of $\hat{K}^{c'} + \hat{K}^{d'}$ in eq. (5.4.32) and $\hat{K}^c + \hat{K}^d$ in eq. (5.4.27), however we **cannot** yet simply add the traces and use the anticommutation relations, since the photon propagators in the two contributions depend on different momenta. However, keep in mind that we still have to convolute these kernels with the wavefunctions $\phi(\vec{p})$ and $\phi(\vec{q})$, and we can after having done that, exchange the names of the dummy momenta $\vec{p} \leftrightarrow \vec{q}$. After this, the photon propagators are the same in the two expressions, and we can add them as we did before:

$$\delta E(\hat{K}^{c} + \hat{K}^{d} + \hat{K}^{c'} + \hat{K}^{d'}) = \int \frac{d^{3}p}{(2\pi)^{3}} \frac{d^{3}q}{(2\pi)^{3}} \frac{d^{4}k}{(2\pi)^{4}} \frac{2e^{4}k^{j}k^{m}}{D(k)D(-k)} \operatorname{Tr}\left[\{\gamma_{i}, \gamma_{m}\}XX^{\dagger}\right] \\ \times \Delta^{ij}(k-q)\Delta^{00}(p-k) \\ \int \frac{d^{3}p}{(2\pi)^{3}} \frac{d^{3}q}{(2\pi)^{3}} \frac{d^{4}k}{(2\pi)^{4}} \frac{2e^{4}k^{j}k^{i}}{D(k)D(-k)} \operatorname{Tr}\left[XX^{\dagger}\right] \\ \times \Delta^{ij}(k-q)\Delta^{00}(p-k).$$
(5.4.33)

Again, we can see the contribution is the same for the singlet and the triplet, so it need not be computed.

5.4.3 Two Coulomb photons

Finally, we need to consider the contribution with two Coulomb photons:



Figure 5.4.7: The contribution with two Coulomb photons.

The trace structure of the crossed diagram and the $K^C S_R K^C$ part of the double exchange will be the same:

$$Tr [(ie\gamma_{0})[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma}](ie\gamma_{0})X \\\times (ie\gamma_{0})[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma}](ie\gamma_{0})X^{\dagger}] \\= Tr [P_{-}(ie\gamma_{0})[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma}](ie\gamma_{0})P_{-}X \\\times P_{+}(ie\gamma_{0})[P_{-}(...) - P_{+}(...) - \vec{k} \cdot \vec{\gamma}](ie\gamma_{0})P_{+}X^{\dagger}]$$
(5.4.34)
$$= Tr [P_{-}(ie\gamma_{0})[P_{-}(E' + k^{0} + m_{e})](ie\gamma_{0})P_{-}X \\\times P_{+}(ie\gamma_{0})[-P_{+}(-E' + k^{0} - m_{e})](ie\gamma_{0})P_{+}X^{\dagger}] \\= -e^{4}(E' + k^{0} + m_{e})(-E' + k^{0} - m_{e}) Tr [XX^{\dagger}]$$

Again, we can see that neither of these diagrams produces any hfs.

5.5 Leading order two loop diagram

Because their evaluation is very lengthy, we will not check all of the two loop diagrams that have to be checked, and instead only present the highest order contribution (references [2,5,6] deal with these diagrams, and the former uses a propagator similar to ours) which is given by the diagram shown on fig. 5.5.1, coming from the $K_R(S_R - S_0)K_R(S_R - S_0)K_R$ part of the kernel correction.

In fact, we will only consider a particular part of this contribution given by

$$K^C S K^T S K^C, (5.5.1)$$

shown on fig. 5.5.2 and we will discuss the other contributions such as

$$K^{C}S_{0}K^{T}S_{0}K^{C} - K^{C}SK^{T}S_{0}K^{C} - K^{C}S_{0}K^{T}SK^{C}$$
(5.5.2)



Figure 5.5.1: The leading order two loop contribution to the hfs.



Figure 5.5.2: The $K^C S K^T S K^C$ part of the contribution.

in the end of this section.

We will call the first relative loop momentum k and the second one k'. Notice that there are two 3-dimensional and two 4-dimensional integrals to be taken here: the \vec{p} and \vec{q} integrals that convolute the kernel with the wavefunction on both sides, and two loop integrals over k and k'. In the case of this diagram, we can immediately evaluate the wavefunction convolution integrals, because as we will see, they will simply follow from the Schrödinger equation.

Let us start with the \vec{p} integral. The only two things that depend on \vec{p} are the wavefunction and the left Coulomb photon propagator, so let us drop everything else for now and consider only these two things:

$$I(\vec{k}) = \int \frac{d^3p}{(2\pi)^3} \frac{i}{|\vec{p} - \vec{k}|^2} \phi(\vec{p}).$$
(5.5.3)

But the Coulomb-Schrödinger equation (eq. (4.2.59)) immediately tells us what the convolution is (in the case of positronium, $m_r = m_e/2$):

$$\frac{d^3 p}{(2\pi)^3} \frac{1}{|\vec{p} - \vec{k}|^2} \phi(\vec{p}) = \left(\frac{\vec{k}^2 + \gamma^2}{m_e e^2}\right) \phi(\vec{k}) \\
= \sqrt{\frac{\gamma^3}{\pi}} \left(\frac{\vec{k}^2 + \gamma^2}{m_e e^2}\right) \frac{4\pi m_e \alpha}{(\vec{k}^2 + \gamma^2)^2} \\
= \sqrt{\frac{\gamma^3}{\pi}} \frac{1}{(\vec{k}^2 + \gamma^2)} \\
I(\vec{k}) = i\sqrt{\frac{\gamma^3}{\pi}} \frac{1}{(\vec{k}^2 + \gamma^2)}$$
(5.5.4)

We can also take the \vec{q} integral in exactly the same way, yielding

$$I(\vec{k}') = \int \frac{d^3q}{(2\pi)^3} \frac{i}{|\vec{k}' - \vec{q}|^2} \phi(\vec{q})$$

= $i\sqrt{\frac{\gamma^3}{\pi}} \frac{1}{(\vec{k}'^2 + \gamma^2)}.$ (5.5.6)

These results are extremely helpful, since they allow us to see that to get the lowest order contribution, we need to only consider the non-relativistic bits of the k and k' loop integrals, since both \vec{k} and $\vec{k'}$ are cut off by $\gamma = m_e \alpha/2$. Recall that we have already approximated the two-particle propagator in the non-relativistic regime in section 4.2.3, we state the result here:

$$\Delta_0^{(1)}(E'\delta_0^{\mu} + k^{\mu})\Delta_0^{(2)}(-E'\delta_0^{\mu} + k^{\mu}) \approx -2\pi i \frac{1}{2E} \frac{(-\not\!\!\!\!/_e + m_e)^{(1)}(\not\!\!\!/_p + m_p)^{(2)}}{\gamma^2 + \vec{k}^2} \,\delta(k^0), \quad (5.5.7)$$

where

$$-P_{e} + m_{e} = P_{-}(E' + m_{e}) - P_{+}(E' - m_{e}) - \vec{k} \cdot \vec{\gamma}$$

$$P_{p} + m_{e} = P_{-}(-E' + m_{e}) - P_{+}(-E' - m_{e}) - \vec{k} \cdot \vec{\gamma}$$
(5.5.8)

Now, with all these considerations in mind, we can compute the energy shift due to this kernel correction:

$$\delta E(CTC) = \frac{i\gamma^3}{4\pi E^2} \int \frac{d^4k}{(2\pi)^4} \frac{d^4k'}{(2\pi)^4} (2\pi\delta(k^0))(2\pi\delta(k'^0)) \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \Delta^{ij}(k - k')$$

$$\times \operatorname{Tr} \left[(ie\gamma_0) \left[P_-(\ldots) - P_+(\ldots) - \vec{k'} \cdot \vec{\gamma} \right] (ie\gamma_i) \left[P_-(\ldots) - P_+(\ldots) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_0) X \right]$$

$$\times (ie\gamma_0) \left[P_-(\ldots) - P_+(\ldots) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_j) \left[P_-(\ldots) - P_+(\ldots) - \vec{k'} \cdot \vec{\gamma} \right] (ie\gamma_0) X^{\dagger} \right]$$

Using the properties of the projectors and spin matrices we have discussed before, the trace can be simplified:

$$\delta E(CTC) = \frac{i\gamma^3}{4\pi E^2} \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \Delta^{ij}(\vec{k} - \vec{k}') \\ \times \operatorname{Tr} \left[(ie\gamma_0) \left[P_-(E' + m_e) - \vec{k}' \cdot \vec{\gamma} \right] (ie\gamma_i) \left[P_-(E' + m_e) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_0) X \\ \times (ie\gamma_0) \left[P_+(E' + m_e) - \vec{k} \cdot \vec{\gamma} \right] (ie\gamma_j) \left[P_+(E' + m_e) - \vec{k}' \cdot \vec{\gamma} \right] (ie\gamma_0) X^{\dagger} \right]$$

Since $\gamma_0 X \gamma_0 = -X$ and $P_- X = X P_+ = X$

$$\delta E(CTC) = -\frac{i\gamma^{3}e^{6}}{4\pi E^{2}} \int \frac{d^{3}k}{(2\pi)^{3}} \frac{d^{3}k'}{(2\pi)^{3}} \frac{1}{(\gamma^{2} + \vec{k}^{2})^{2}} \frac{1}{(\gamma^{2} + \vec{k}^{\prime 2})^{2}} \Delta^{ij}(\vec{k} - \vec{k}') \\ \times \operatorname{Tr}\left[P_{-}\left([E' + m_{e}] - \vec{k}' \cdot \vec{\gamma}\right)\gamma_{i}\left([E' + m_{e}] - \vec{k} \cdot \vec{\gamma}\right)P_{-}X \\ \times P_{+}\left([E' + m_{e}] - \vec{k} \cdot \vec{\gamma}\right)\gamma_{j}\left([E' + m_{e}] - \vec{k}' \cdot \vec{\gamma}\right)P_{+}X^{\dagger}\right]$$
(5.5.9)

Where we have again used the property of X to get the projectors out to make the next step clear. Since an odd number of spatial gamma matrices sandwiched between two same projectors vanishes:

$$\delta E(CTC) = -\frac{i\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \Delta^{ij}(\vec{k} - \vec{k}') \\ \times \operatorname{Tr}\left[\left[(\vec{k}' \cdot \vec{\gamma})\gamma_i + \gamma_i(\vec{k} \cdot \vec{\gamma}) \right] X \left[(\vec{k} \cdot \vec{\gamma})\gamma_j + \gamma_j(\vec{k}' \cdot \vec{\gamma}) \right] X^{\dagger} \right]$$
(5.5.10)

Proceed by simplifying the following expression in the trace:

$$(\vec{k}' \cdot \vec{\gamma})\gamma_i + \gamma_i(\vec{k} \cdot \vec{\gamma}) = k'^m \gamma_m \gamma_i + \gamma_i(\vec{k} \cdot \vec{\gamma})$$

= $k'^m (-2\delta_{im} - \gamma_i \gamma_m) + \gamma_i(\vec{k} \cdot \vec{\gamma})$ (5.5.11)
= $-2k'_i + \gamma_i(\vec{\ell} \cdot \vec{\gamma})$

where we have defined $\vec{\ell} = \vec{k} - \vec{k'}$. As we have seen in previous sections, it can be very advantageous to exploit the innate symmetry of these equations, so why commute the $\vec{k'}$ term and not the \vec{k} ?

$$(\vec{k}' \cdot \vec{\gamma})\gamma_i + \gamma_i(\vec{k} \cdot \vec{\gamma}) = (\vec{k}' \cdot \vec{\gamma})\gamma_i + k^m \gamma_i \gamma_m$$

= $(\vec{k}' \cdot \vec{\gamma})\gamma_i + k^m (-2\delta_{im} - \gamma_m \gamma_i)$
= $-2k_i - (\vec{\ell} \cdot \vec{\gamma})\gamma_i$ (5.5.12)

We can now add the expressions to obtain a symmetrized version

$$(\vec{k}' \cdot \vec{\gamma})\gamma_i + \gamma_i(\vec{k} \cdot \vec{\gamma}) = -(k_i + k_i') + \frac{1}{2} [\gamma_i, \vec{\ell} \cdot \vec{\gamma}], \qquad (5.5.13)$$

doing this leaves us with four terms in the trace:

$$\operatorname{Tr}\left[\left(-(k_{i}+k_{i}')+\frac{1}{2}[\gamma_{i},\vec{\ell}\cdot\vec{\gamma}]\right)X\left(-(k_{j}+k_{j}')-\frac{1}{2}[\gamma_{j},\vec{\ell}\cdot\vec{\gamma}]\right)X^{\dagger}\right]$$

$$=(k_{i}+k_{i}')(k_{j}+k_{j}')\operatorname{Tr}[XX^{\dagger}]$$

$$-\frac{1}{2}(k_{j}+k_{j}')\operatorname{Tr}\left[[\gamma_{i},\vec{\ell}\cdot\vec{\gamma}]XX^{\dagger}\right]+\frac{1}{2}(k_{i}+k_{i}')\operatorname{Tr}\left[X[\gamma_{j},\vec{\ell}\cdot\vec{\gamma}]X^{\dagger}\right]$$

$$-\frac{1}{4}\operatorname{Tr}\left[[\gamma_{i},\vec{\ell}\cdot\vec{\gamma}]X[\gamma_{j},\vec{\ell}\cdot\vec{\gamma}]X^{\dagger}\right].$$
(5.5.14)

Notice that the first term cannot contribute to the hfs, so we ignore it from now on. Since the variables \vec{k} and $\vec{k'}$ are dummy, we can rename $\vec{k} \leftrightarrow \vec{k'}$, which does not affect any terms in the integrand that are outside of the trace (the transverse photon is even in momentum). However, the second and third term in the trace change sign since under this transformation $\vec{\ell} \leftrightarrow -\vec{\ell}$, such that their integral vanishes. This means that we only need to consider the last term.

$$\delta E(CTC) = \frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \frac{1}{\vec{\ell}^2} \left(\delta^{ij} - \frac{\ell^i \ell^j}{\vec{\ell}^2} \right) \\ \times \frac{1}{4} \operatorname{Tr} \Big[[\gamma_i, \vec{\ell} \cdot \vec{\gamma}] X [\gamma_j, \vec{\ell} \cdot \vec{\gamma}] X^{\dagger} \Big]$$
(5.5.15)

$$\delta E(CTC) = \frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{\ell_k \ell_m}{\vec{\ell}^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \times \frac{1}{4} \operatorname{Tr} \left[[\gamma_i, \gamma_k] X[\gamma_i, \gamma_m] X^{\dagger} \right]$$
(5.5.16)

$$[\gamma_i, \gamma_k] = \begin{pmatrix} -[\sigma_i, \sigma_k] & 0\\ 0 & -[\sigma_i, \sigma_k] \end{pmatrix} = -2i\varepsilon_{ika} \begin{pmatrix} \sigma_a & 0\\ 0 & \sigma_a \end{pmatrix}$$
(5.5.17)

$$\delta E(CTC) = -\frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{\ell_k \ell_m}{\vec{\ell}^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \times \varepsilon_{ika} \varepsilon_{imb} \operatorname{Tr} \left[\sigma_a \xi \sigma_b \xi^{\dagger} \right]$$
(5.5.18)

At this point, let us calculate the shifts for the singlet and triplet separately. Starting with the singlet, for which $\xi^{00} = \frac{1}{\sqrt{2}}$

$$\delta E^{00}(CTC) = -\frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{\ell_k \ell_m}{\vec{\ell}^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \\ \times \frac{1}{2} (\delta_{km} \delta_{ab} - \delta_{kb} \delta_{am}) \operatorname{Tr}[\sigma_a \sigma_b] \\ = -2 \frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \\ = -2 \frac{e^6 (E' + m_e)^2}{4E^2 (8\pi\gamma)^2} |\phi(\vec{0})|^2$$

$$(5.5.19)$$

Substituting the values for γ and E', at leading order we get

$$\delta E^{00}(CTC) = -\left(\frac{E' + m_e}{E}\right)^2 \frac{m_e \alpha^4}{4} \approx -\frac{m_e \alpha^4}{4}$$
(5.5.20)

Whereas for the triplet $\xi^{1m}=\frac{1}{\sqrt{2}}\vec{\epsilon}\cdot\vec{\sigma}$

$$\delta E^{1m}(CTC) = -\frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}^2)^2} \frac{\ell_k \ell_m}{\vec{\ell}^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \\ \times \frac{1}{2} (\delta_{km} \delta_{ab} - \delta_{kb} \delta_{am}) \epsilon_c \epsilon_d^* \operatorname{Tr}[\sigma_a \sigma_c \sigma_b \sigma_d] \\ = -\frac{\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2} \int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \frac{1}{\vec{\ell}^2} \frac{1}{(\gamma^2 + \vec{k}'^2)^2} \\ \times \frac{1}{2} (\vec{\ell}^2 \operatorname{Tr}[\sigma_a \sigma_c \sigma_a \sigma_d] - \ell_k \ell_m \operatorname{Tr}[\sigma_m \sigma_c \sigma_k \sigma_d]) \epsilon_c \epsilon_d^*$$
(5.5.21)

$$= -\frac{\gamma^{3}e^{6}(E'+m_{e})^{2}}{4\pi E^{2}} \int \frac{d^{3}k}{(2\pi)^{3}} \frac{d^{3}k'}{(2\pi)^{3}} \frac{1}{(\gamma^{2}+\vec{k}^{2})^{2}} \frac{1}{\vec{\ell}^{2}} \frac{1}{(\gamma^{2}+\vec{k}'^{2})^{2}} \times \left(\vec{\ell}^{2}(\delta_{ac}\delta_{ad}-\delta_{aa}\delta_{cd}+\delta_{ad}\delta_{ca})-\ell_{k}\ell_{m}(\delta_{mc}\delta_{kd}-\delta_{mk}\delta_{cd}+\delta_{md}\delta_{ck})\right)\epsilon_{c}\epsilon_{d}^{*}$$
(5.5.22)
$$= \frac{2\gamma^{3}e^{6}(E'+m_{e})^{2}}{4\pi E^{2}} \int \frac{d^{3}k}{(2\pi)^{3}} \frac{d^{3}k'}{(2\pi)^{3}} \frac{1}{(\gamma^{2}+\vec{k}^{2})^{2}} \frac{(\vec{\ell}\cdot\vec{\epsilon})(\vec{\ell}\cdot\vec{\epsilon}^{*})}{\vec{\ell}^{2}} \frac{1}{(\gamma^{2}+\vec{k}'^{2})^{2}}$$

Now all that remains is to take this integral, for which we use the convolution theorem. The theorem goes as follows: given three functions $g(\vec{x})$, $f(\vec{x})$, $h(\vec{x})$ and their Fourier transforms, for their convolution, we have

$$\int \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} g(\vec{k}) f(\vec{k} - \vec{k'}) h(\vec{q}) = \int d^3x \ g(\vec{x}) f(-\vec{x}) h(-\vec{x}).$$
(5.5.23)

For this particular case, both $g(\vec{p})$ and $h(\vec{q})$ are simply equal to the ground state wavefunction, and $f(\vec{x})$ can be found by performing a Fourier transformation:

$$f(\vec{x}) = \epsilon_i \epsilon_j^* \int \frac{d^3 \ell}{(2\pi)^3} \frac{\ell_i \ell_j}{\vec{\ell}^2} e^{i\vec{\ell}\cdot\vec{x}}$$

$$= -\epsilon_i \epsilon_j^* \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \int \frac{d^3 \ell}{(2\pi)^3} \frac{1}{\vec{\ell}^2} e^{i\vec{\ell}\cdot\vec{x}},$$
(5.5.24)

so that we can simply take derivatives of the Coulomb potential to find $f(\vec{x})$

$$f(\vec{x}) = -\frac{\epsilon_i \epsilon_j^*}{4\pi} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \left(\frac{1}{r}\right)$$

$$= \frac{1}{4\pi r^3} \left((\vec{\epsilon} \cdot \vec{\epsilon^*}) - \frac{3(\vec{\epsilon} \cdot \vec{x})(\vec{\epsilon^*} \cdot \vec{x})}{r^2} \right) + \frac{1}{3} \delta(\vec{r})(\vec{\epsilon} \cdot \vec{\epsilon^*})$$
(5.5.25)

At this point it should be clear that this is precisely the calculation done in quantum mechanics: this expression is nothing but the expectation value of the dipole field produced by the "nucleus" interacting with the "electron" spin.

The first part of eq. (5.5.25) is concerning, because it looks like it might potentially split the triplet itself (produce different energy shifts for different polarizations), which is not something we expect. However, as we will now demonstrate, this contribution simply vanishes. Let us use the convolution theorem as well as eq. (5.2.2) to reduce the six-dimensional integral to a 3-dimensional one:

$$\delta E^{1m}(CTC) = \frac{2\gamma^3 e^6 (E' + m_e)^2}{4\pi E^2 (8\pi\gamma)^2} \int d^3x \, e^{-2\gamma r} \left[\frac{1}{4\pi r^3} \left(1 - \frac{3(\vec{\epsilon} \cdot \vec{x})(\vec{\epsilon^*} \cdot \vec{x})}{r^2} \right) + \frac{1}{3}\delta(\vec{r}) \right]$$

However, for any two vectors \vec{a} and \vec{b}

$$\int d\Omega \ (\vec{a} \cdot \hat{r})(\vec{b} \cdot \hat{r}) = \frac{4\pi}{3}(\vec{a} \cdot \vec{b}), \qquad (5.5.26)$$

so that indeed, the first part of the integral vanishes:

$$\int d\Omega \left(1 - \frac{3(\vec{\epsilon} \cdot \vec{x})(\vec{\epsilon}^* \cdot \vec{x})}{r^2}\right) = 0.$$
(5.5.27)

Substituting the values for γ and E', at leading order we get

$$\delta E^{1m}(CTC) = \left(\frac{E' + m_e}{E}\right)^2 \frac{m_e \alpha^4}{12} \approx \frac{m_e \alpha^4}{12}$$
(5.5.28)

Finally, combining eq. (5.5.20) and eq. (5.5.28), we get the leading order hfs contribution coming from this diagram:

$$\delta E^{1m}(CTC) - \delta E^{00}(CTC) = \frac{m_e \alpha^4}{3}.$$
 (5.5.29)

5.5.1 More cancellations

Let us return to the parts of the $K^C(S_R - S_0)K^T(S_R - S_0)K^C$ that we disregarded in the last section, eq. (5.5.2):

$$K^{C}S_{0}K^{T}S_{0}K^{C} - K^{C}SK^{T}S_{0}K^{C} - K^{C}S_{0}K^{T}SK^{C}.$$
(5.5.30)

The simplest of these is the first term. Notice that the transverse photon is placed between two reference propagators S_0 . However, the electron (positron) line of S_0 contains the projector P_- (P_+), which leads to the transverse photon vertices to be left between two of the same projector:

$$[P_{-}(ie\gamma_{i})P_{-}]^{(1)}[P_{+}(ie\gamma_{j})P_{+}]^{(2)} = 0, \qquad (5.5.31)$$

so that this contribution vanishes.

As for the other two contributions, we should first use the Coulomb-Schrödinger equation (in its abstract form) to simplify them. The equation is

$$S_0 K_0 \Psi^0 = \Psi^0 \tag{5.5.32}$$

with its conjugate

$$\bar{\Psi}^0 = \bar{\Psi}^0 K_0 S_0. \tag{5.5.33}$$

Here, the reference kernel K_0 is approximately the Coulomb interaction, given by

$$K_0 = \frac{1}{N}K^C, \qquad N = \frac{(E' + m_e)^2}{4E'm_e} \approx 1.$$
 (5.5.34)

But this lets us simplify the energy contributions from the second and third term in eq. (5.5.30):

$$-\bar{\Psi}^{0}K^{C}SK^{T}\underbrace{S_{0}K^{C}\Psi^{0}}_{N\Psi^{0}} - \underbrace{\bar{\Psi}^{0}K^{C}S_{0}}_{N\bar{\Psi}^{0}}K^{T}SK^{C}\Psi^{0}$$

$$= -N\bar{\Psi}^{0}K^{C}SK^{T}\Psi^{0} - N\bar{\Psi}^{0}K^{T}SK^{C}\Psi^{0}.$$
(5.5.35)



Figure 5.5.3: Contributions from $K_R(S_R - S_0)K_R$.

As one can see, these are exactly the corrections considered in section 5.4.2. The reason we do not consider them here, is because they need to be combined with the corrections shown on fig. 5.5.3. In these corrections, the blob can either be S (which we expect to give higher order corrections) or S_0 . The S_0 part combines with the contributions from eq. (5.5.35) in exactly the same manner as in section 5.4.2.

Considering all these cancellations, calls for a further rearrangement of the perturbation expansion, so at to make these more explicit. It seems possible to obtain an expansion similar to that of [2] rather than [1,6], but since we do not consider higher order corrections, we do not pursue this further.

Chapter 6

Conclusion

For positronium we confirm the well known result for the hfs at leading order, there are two contributions – the Fermi splitting and the annihilation correction

$$\Delta E_{hfs} \approx \frac{m_e \alpha^4}{3} + \frac{m_e \alpha^4}{4} = \frac{7m_e \alpha^4}{12}.$$

However, in its current state the calculation scheme presented here is not suitable for computing higher order corrections. In order to go to higher orders one of two things can done. We have mentioned several times that cancellations such as the ones presented in section 5.5.1 point to a possible rearrangement of the perturbation expansion. Most probably, the perturbation expansion used in [2] will be more suitable to use with the reference propagator we currently have.

Another way to go about this is to change the propagator itself. Notice that the compensating kernel correction is proportional to the difference of propagators (the bare one and the reference propagator). Which means that the simpler the propagator, the more compensating corrections there are. So picking a more complicated propagator that is less non-relativistic, would make for a simpler kernel. Of course this does not come for free, since the reference equation (the Schrödinger equation in our case) is dictated by the reference propagator, so a more complicated propagator leads to a more complicated wavefunction. However in our experience, judging from the works [1] and [6] it is easier to deal with a more complex wavefunction than a more complex kernel.

Appendix A Notation

A.1 Momentum convolution

The BSE with the Dirac indices suppressed is:

$$G(P; p, q) = S(P; p) + \int \frac{d^4k}{(2\pi)^4} S(P; p) K(P; p, k) G(P; k; q),$$
(A.1.1)

where P is the total momentum, p is the relative momentum of incoming particles and q is the relative momentum of the outgoing particles. Normally, we write the equation as follows:

$$G(P; p; q) = S(P; p) + S(P; p)K(P; p, k)G(P; k, q),$$
(A.1.2)

where the integration over intermediate relative momenta are implicit.

A.2 Dirac indices

The Dirac indices are also generally suppressed. To express how, let us consider the simplest contribution to the 4-point GF in QED – single exchange.



It is obvious from this example that the GF will depend on four Dirac indices. We will express that as $G_{ab;cd}$, where the first two indices a, b (c, d) stand for the Dirac indices of

the incoming (outgoing) electron and the anti-particle, respectively. Let us now consider the GF for single exchange:

$$G_{ab;cd}^{s.p.} = \left[\Delta_{cg}^{(1)} \left(ie\gamma^{\mu}\right)_{ge}^{(1)} \Delta_{ea}^{(1)}\right] \Delta_{\mu\nu} \left[\Delta_{bf}^{(2)} \left(ie\gamma^{\nu}\right)_{fh}^{(2)} \Delta_{hd}^{(2)}\right].$$
(A.2.1)

We rearrange this to bring into the form required for the Dyson equation:

$$G_{ab;cd}^{s.p.} = \Delta_{ea}^{(1)} \Delta_{bf}^{(2)} \left(\left(i e \gamma^{\mu} \right)_{ge}^{(1)} \Delta_{\mu\nu} \left(i e \gamma^{\nu} \right)_{fh}^{(2)} \right) \Delta_{cg}^{(1)} \Delta_{hd}^{(2)}$$

= $S_{ab;ef}$ $K_{ef;gh}^{s.p.}$ $S_{gh;cd}$, (A.2.2)

where we have defined:

$$S_{ab;ef} = \Delta_{ea}^{(1)} \Delta_{bf}^{(2)} \qquad K_{ef;gh}^{s.p.} = (ie\gamma^{\mu})_{ge}^{(1)} \Delta_{\mu\nu} (ie\gamma^{\nu})_{fh}^{(2)}$$
(A.2.3)

We would generally suppress the Dirac indices in eq. (A.2.2), and write it as

$$G^{s.p.} = \Delta^{(1)} \Delta^{(2)} \left(\left(i e \gamma^{\mu} \right)^{(1)} \Delta_{\mu\nu} \left(i e \gamma^{\nu} \right)^{(2)} \right) \Delta^{(1)} \Delta^{(2)}.$$
(A.2.4)

The Dyson equation with the Dirac indices explicit, but the momentum convolution suppressed is:

$$G_{ab;cd} = S_{ab;cd} + S_{ab;ef} K_{ef;gh} G_{gh;cd}, \tag{A.2.5}$$

suppressing the matrix multiplication,

$$G = S + SKG \tag{A.2.6}$$

Appendix B

Conventions

 $\hbar = 1$ c = 1

 $\eta_{\mu\nu} \leftrightarrow \text{diag}(-1, 1, 1, 1)$

Fourier transforms

$$f(k) = \int d^n x e^{-ik \cdot x} f(x) \qquad f(x) = \frac{1}{(2\pi)^n} \int d^n k e^{ik \cdot x} f(k)$$

Fourier transform of the Green's function:

$$G(p_1, p_2, \dots, p_n) = \int dx_1 \dots dx_n \, e^{-ip_1 x_1} \dots e^{-ip_n x_n} \left\langle \Omega \right| T\phi(x_1) \dots \phi(x_n) \left| \Omega \right\rangle$$

Canonical commutation relations for a scalar field:

$$[\phi(\vec{x},t),\phi(\vec{y},t)] = 0 \qquad [\phi(\vec{x},t),\partial_t\phi(\vec{y},t)] = i\delta(\vec{x}-\vec{y})$$

Coulomb-Schrödinger equation in momentum space

$$\left(\frac{\vec{p}^{\,2}}{2m} - E\right)\Psi(\vec{p}\,) = \int \frac{d^3q}{(2\pi)^3} \frac{e^2}{|\vec{p} - \vec{q}\,|^2}\,\Psi(\vec{q}\,)$$

Gamma matrices

$$\{\gamma_{\mu}, \gamma_{\nu}\} = -2\eta_{\mu\nu} \qquad (-i\gamma_{\mu}\partial^{\mu} + m)\Psi = 0$$
$$\gamma^{0} = \begin{pmatrix} 1 & 0\\ 0 & -1 \end{pmatrix} \qquad \gamma^{1} = \begin{pmatrix} 0 & \sigma_{1}\\ -\sigma_{1} & 0 \end{pmatrix} \qquad \gamma^{2} = \begin{pmatrix} 0 & \sigma_{2}\\ -\sigma_{2} & 0 \end{pmatrix} \qquad \gamma^{3} = \begin{pmatrix} 0 & \sigma_{3}\\ -\sigma_{3} & 0 \end{pmatrix}$$
Pauli matrices

 $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

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