Relativistic bound states in Yukawa theory

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Abstract. A generalization of the Gell-Mann–Low Theorem is applied to bound state
calculations in Yukawa theory with a massless boson. The resulting effective Schrödinger
equation is solved both numerically and perturbatively around the non-relativistic limit. I
discuss the spectrum and compare with the case of quantum electrodynamics.

1. Introduction

Bound state calculations in relativistic quantum field theories have a long history. Its beginning
is marked by the formulation of the Bethe-Salpeter equation[1, 2]. Soon after its formulation it
became clear that solving the Bethe-Salpeter equation is a difficult endeavor, because of technical
difficulties as well as conceptual problems (for an overview see, e.g.[3]). A great variety of
different approaches have been developed since that time, the most important of which I have
tried to resume in[4].

In recent years, a new approach to the bound state problem has been formulated[5] which
avoids at least many of the shortcomings of the Bethe-Salpeter approach. It is based on a
generalization of the Gell-Mann–Low theorem[2]. The new formalism has been successfully
applied[6] to the Wick-Cutkosky model. In the present contribution, I will go one step further
and test this technique on Yukawa theory.

The description of bound states in Yukawa theory has turned out to be notoriously difficult.
The solution of the Bethe-Salpeter equation is plagued by the complications due to the spinor
structure and, more importantly, the fact that the integral kernel in the equation is not
of Fredholm type. As a consequence, from analytical considerations practically nothing is
known about the solutions, they might not even exist[7]. Direct numerical solutions have been
attempted. However, the singular nature of the integral equation forces the introduction of an
arbitrary UV cutoff, and resulting solutions depend sensibly on this unphysical cutoff[8].

In more recent times, calculations in light-front quantization have been performed for Yukawa
theory, both in a Tamm-Dancoff approximation[9] and in covariant light-front dynamics[10]. In
the end, problems similar to the ones with the Bethe-Salpeter equation arise also in these
approaches. I have not been able to find other bound state calculations in Yukawa theory
in the literature. However, the application of quasipotential equations[11] may be free of
inconsistencies. In any case, the results presented here (or similar results for a possible
comparison) have not been obtained, to the best of my knowledge, by any method before.

In this contribution, I will show that the application of the generalized Gell-Mann–Low
theorem is straightforward and completely free of inconsistencies. For the calculation of the
bound state spectrum, I will focus on the case of massless boson exchange, for three reasons. First, the massless case is the most singular one, hence if the formalism works in this case, it is expected to be applicable to the case of a massive boson as well. Second, the massless case allows for an analytical calculation of the first relativistic corrections, i.e., the fine and hyperfine structure. Finally, in this case, in the non-relativistic limit, the problem reduces to two fermions interacting through an instantaneous Coulomb potential, and it is interesting to compare the fine and hyperfine structure with the corresponding ones for massless vector boson exchange (electrodynamic interaction).

The organization of this contribution is as follows: in the next section, I will determine the effective or Bloch-Wilson Hamiltonian to lowest non-trivial order, which will be the starting point for all the following calculations. In Section 3 and 4, the numerical and analytical results for the spectrum are presented and discussed.

2. The Bloch-Wilson Hamiltonian

The generalized Gell-Mann–Low theorem is derived in[5] and its application to bound state problems illustrated in[6]. For our present purposes, it is sufficient to remark that the effective Hamiltonian for the constituents of a bound state arises from “integrating out” the additional degrees of freedom within a Hamiltonian formalism, in a way similar to a Born-Oppenheimer approximation.

This formalism will be applied here to Yukawa theory. To simplify matters, we consider two different fermion species, A and B, which interact with a scalar boson. Hence the Hamiltonian of the theory consists of the free Hamiltonians for the fermions A and B and the scalar boson, and the interaction term

$$ g \int d^3x \left( \bar{\psi}_A \psi_A + \bar{\psi}_B \psi_B \right) \phi. \tag{1} $$

We are interested in bound states of one fermion A and one fermion B. (Other bound states, of identical fermions or fermion and antifermion, e.g., in a theory with only one fermion species, are simply related to bound states of type AB and can be treated by exactly the same method.) The application of the generalized Gell-Mann–Low theorem to lowest non-trivial order leads to the following effective time-independent Schrödinger equation in the c.m.s.:

$$ \left( \sqrt{m_A^2 + p^2} + \sqrt{m_B^2 + p'^2} \right) \phi(p) - g^2 \int \frac{d^3p'}{(2\pi)^3} \left( \sum_{A,B} \frac{E_A + m_A}{2E'_p} \frac{E_B + m_B}{2E'_p} \right) \left[ \frac{E_A + m_A}{E'_p} + \frac{E_B + m_B}{E'_p} \right] \phi(p') = E\phi(p). \tag{2} $$

Here $p = p_A = -p_B$ is the relative momentum, $m_A$ and $m_B$ represent the one-loop renormalized masses, the relativistic kinetic energies are denoted by

$$ E_p^A = \sqrt{m_A^2 + p^2}, \quad \omega_p = \sqrt{\mu^2 + p^2} \tag{3} $$

($\mu$ is the mass of the scalar boson), $E$ is the (rest frame) energy of the two-particle state minus the one-loop renormalized vacuum energy, and the wavefunction $\phi(p)$ in a spinorial representation is related to the eigenstate $\phi$ in the space of all states of the (free) particles A and B via

$$ \phi(p) = \sum_{r,s} \langle 0 | a_B(-p,s) a_A(p,r) | \phi \rangle \chi_A(r) \otimes \chi_B(s). \tag{4} $$
Here $\chi_A(r)$ is a Pauli spinor, normalized in the common (non-relativistic) sense, which describes the orientation $(r)$ of the spin of fermion $A$. As usual, $\sigma_A$ is understood to act on $\chi_A(r)$ only.

3. Numerical solution

In order to actually solve the effective Schrödinger equation (2), one first separates the angular and spin degrees of freedom. The effective Hamiltonian is rotationally invariant, hence it is natural to consider total angular momentum eigenstates. To make contact to the usual spectroscopy, I choose to couple first the individual spins to a total spin $S$ and then couple this spin with the relative orbital angular momentum $L$ to the total angular momentum $J$. The well-known construction with Clebsch-Gordan coefficients yields simultaneous eigenfunctions of $J^2$, $J_z$, $S^2$, and $L^2$.

For a given $l$, $J$ can take the values $l$ (for $S = 0$) and $l, l + 1$ (for $S = 1$, provided $l \neq 0$). The effective Hamiltonian conserves the total angular momentum $J$ and spatial parity $(-1)^l$, but a priori not $S$ nor $l$. As a consequence, one finds that the effective Schrödinger equation decays into pairs of coupled one-dimensional integral equations (in $p \equiv |p|$). For a given value of $J \neq 0$, the equations for $l = J, S = 0$ and $l = J, S = 1$ are coupled (“$S$-coupling”), as are the equations for $l = J - 1, S = 1$ and $l = J + 1, S = 1$ (“$l$-coupling”). In the special case $J = 0$, the two possible angular momentum eigenstates are uncoupled.

The remaining (pairs of) one-dimensional integral equations can now be solved numerically.

In practice, we have approximated the solutions by a finite linear combination of an appropriately chosen set of up to 40 basis functions.

The whole procedure outlined above can be carried through independently of the boson mass $\mu$. In what follows, I will focus on the case of massless bosons, as discussed in the introduction. The numerical solutions for $\mu = 0$ are shown in Figs. 1 and 2 for two extreme mass ratios, $m_A = m_B$ and $m_B \rightarrow \infty$ (with $m_A$ fixed), as functions of (the analogue of) the fine structure constant $\alpha = g^2/4\pi$. Between these two extremes, the eigenvalues for fixed $\alpha$ can be seen to vary smoothly with the mass ratio. In Figs. 1 and 2, the energy eigenvalues are normalized to twice the non-relativistic ionization energy for the case of a Coulomb potential, $m_e\alpha^2$, with the reduced mass $m_r$. In the weak-coupling limit $\alpha \rightarrow 0$, the energies tend to the non-relativistic Coulomb values $-m_e\alpha^2/(2n^2)$, $n = 1, 2, 3, \ldots$, as expected for $\mu = 0$.

I begin by discussing the equal-mass case Fig. 1. The binding is weaker in this case than predicted by the non-relativistic formula. Since the masses are equal, the effective Hamiltonian possesses an additional symmetry under the exchange of the fermions $A$ and $B$. Together with the symmetry under spatial parity, this new symmetry forbids $S$-coupling, hence $S$ becomes a good quantum number in this case. Even though the eigenvalues are the same in the non-relativistic limit, the sign of the relativistic corrections is opposite to the case of an electromagnetic interaction (exchange of photons). Also, the ordering of the levels is different.

In the one-body limit $m_B \rightarrow \infty$ depicted in Fig. 2, the sign of the relativistic corrections is different from the equal-mass case. There are always two states exactly degenerate (within the numerical accuracy). The reason can be seen from the effective Schrödinger equation (2). When taking the limit $m_B \rightarrow \infty$, the spin of fermion $B$ dynamically decouples, so that the energy becomes independent of the orientation of $s_B$. The total angular momentum of fermion $A$, $j_A = L + s_A$, becomes a conserved quantity. Together with the invariance under spatial parity, this implies that the orbital angular momentum $l$ is a good quantum number in this limit. Unlike for the Dirac equation with an electromagnetic Coulomb potential, states with the same $j_A$ but different $l$ are not degenerate. In addition, the ordering of the $l = 1$ states is opposite to the electromagnetic case.
4. Fine and hyperfine structure

The effective Hamiltonian in Eq. (2) can be expanded in powers of $p/m_A$, $p'/m_A$, $p/m_B$, and $p'/m_B$ around the non-relativistic limit, to calculate the first relativistic corrections. The result of this expansion is, for the case $\mu = 0$,

$$
\left[ \frac{p^2}{2m_r} - \left( \frac{1}{m_A} + \frac{1}{m_B} \right) \frac{p^4}{8} \right] \phi(p) - g^2 \int \frac{d^3p'}{(2\pi)^3} \frac{1}{|p - p'|^2} \left[ 1 - \frac{p^2 - p'^2}{4m_r|p - p'|} \right] \phi(p') - \left( \frac{1}{m_A} + \frac{1}{m_B} \right) \left( \frac{p^2 + p'^2}{8} - \frac{(p^2 - p'^2)^2}{8|p - p'|^2} - \left( \frac{(p \cdot \sigma_A)(p' \cdot \sigma_A)}{4m_A^2} + \frac{(p \cdot \sigma_B)(p' \cdot \sigma_B)}{4m_B^2} \right) \right) \phi(p')
$$

$$
= (E - m_A - m_B)\phi(p).
$$

The leading order in this expansion gives the non-relativistic Schrödinger equation with a Coulomb potential in momentum space (compare with the numerical solutions in the limit $\alpha \to 0$). The relativistic correction terms are of relative order $p^2/m^2$ and hence give contributions of the relative order $\alpha^2$, with the exception of the first correction term in the potential (last term in the first line of Eq. (5)) which is formally of relative order $p/m$. However, this term is antihermitian and its contribution to relative order $\alpha$ vanishes. Nevertheless, it may contribute to order $\alpha^2$ through second-order perturbation theory. I will not take this contribution into account in the following. From a comparison with the numerical solutions we expect that it should be very small.

To evaluate the contributions of the other, hermitian, correction terms, one uses quantum-mechanical time-independent perturbation theory. Not for all of the terms the contributions are known from the corresponding calculations for hydrogen and positronium. Due to a sign change in the spin-dependent term, (a part of) this term does not combine with the first hermitian correction term in the potential to the Darwin term as it would in the case of an electromagnetic interaction. In addition, the second hermitian correction term in the potential (second term in the second line of Eq. (5)) stems from the retardation of the interaction through scalar boson exchange and is absent in the electromagnetic case. The corresponding contributions have been evaluated directly in momentum space.

To give a flavor of the results, I will present the explicit expressions for the two lowest-lying states, individually for the different hermitian correction terms in Eq. (5) (including the relativistic correction to the kinetic energy), in the order they appear there. The energy corrections turn out to be identical for the states $1^1S_0$ and $1^3S_1$ (in the spectroscopic notation $n^2S_{\frac{1}{2}}L_{\frac{1}{2}}$), and evaluate to

$$
-\frac{5}{8} \left( \frac{1}{m_A^2} + \frac{1}{m_B^2} \right) m_4 \alpha^4 + \left( \frac{3}{4} - \frac{1}{2} + \frac{1}{4} \right) \left( \frac{1}{m_A^2} + \frac{1}{m_B^2} \right) m_4 \alpha^4.
$$

As an immediate consequence, we have the absence of hyperfine splitting for the ground state, to relative order $\alpha^2$. Furthermore, Eq. (6) shows the sign change of the correction term when varying the mass ratio from equal masses $m_r = m_A/2 = m_B/2$ to the one-body limit $m_r = m_A$, $1/m_B = 0$.

The result for the states $2^1S_0$ and $2^3S_1$ is very similar, in particular, there is no hyperfine structure for these states, either. The states $2^1P_1$ and $2^3P_1$ are $S$-coupled through non-diagonal matrix elements in the non-relativistically degenerate $n = 2$ subspace. In the one-body limit, the approximate eigenstates become degenerate with the states $2^3P_0$ and $2^3P_2$, respectively. Close to the one-body limit, there is again no hyperfine structure to order $m_A(m_A/m_B)\alpha^4$, which appears, however, for these states at relative order $(m_A/m_B)^2\alpha^2$. 

$$
\text{and } 2^3S_1. 
$$
In the limit of equal masses, the $S$-coupling disappears. The three states $2^1S_0$, $2^3S_1$, and $2^3P_0$ become degenerate to this order, and the four states $2^3P_0$, $2^3P_1$, $2^1P_1$, and $2^3P_2$ (in the order of descending energy) are equally spaced, which is very nicely reflected by the numerical results in Fig. 1.

In summary, we find a completely consistent picture for the bound state spectrum (and the states themselves) in Yukawa theory through the application of the generalized Gell-Mann–Low theorem. Abnormal solutions or problems with the one-body limit are absent. All qualitative features of the spectrum can already be deduced from a calculation of the first relativistic corrections. There is no hyperfine structure, which corresponds to the absence of a direct spin-spin interaction. Due to the different sign of the spin-dependent relativistic correction term, the overall signs of the relativistic corrections and the level ordering of the $l = 1$ states are different from the case of an electromagnetic interaction. Unlike for the electromagnetic case, there is an important contribution from the retardation of the interaction, which is responsible for the lifting of the degeneracy in $l$. A possible additional contribution from an antihermitian term in the effective Hamiltonian, also related to retardation, has not been evaluated here. A comparison of the numerical results with the analytical values of the other relativistic corrections suggests that this contribution should be very small.

**Figure 1.** The lowest eigenvalues of the effective Hamiltonian as functions of the coupling constant, for the case of equal fermion masses.
Figure 2. The lowest energy eigenvalues in the one-body limit \( m_B \to \infty \).

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