APPENDIX F

Transition Matrix Elements and Matching to an Effective Field Theory

In this appendix we will investigate matrix elements associated with transitions between bound states mediated by the electromagnetic 4-current $J^\mu(x)$ in scalar QED. The motivation for doing this is 2-fold, first to study bound state dynamics which may be applicable to black hole binaries in an effective field theory, and second to see how an effective field theory is constructed and matched to a full UV theory.

F.1. Investigating Matrix Elements

F.1.1. Transitions Mediated by the Electromagnetic Current, J^μ

The matrix element

$$\left\langle n'\ell'm' \right| J^\mu(0) \left| n\ell m \right\rangle \tag{F.1}$$

represents possible transitions between the state $|n'\ell'm'\rangle$ and $|n\ell m\rangle$ mediated by electromagnetic current (and charge density, of course) at the origin. In particular, when this matrix element is nonzero we may physically interpret it to mean that a transition between the states is possible and will result in some nonzero expectation value of J^μ at the origin.

F.1.2. Selection Rules

We can anticipate which quantum numbers will change or not under transitions mediated by J^μ based on it's structure.

Since J contains information about J^0 is a rank-0 tensor and is even under parity. Therefore, transitions mediated by this component must follow $(-1)^{\ell'} = (-1)^{\ell}$. The other component of the 4-vector, $\vec{J}$, is a rank-1 tensor and is odd under parity. Transitions mediated by this component must satisfy $(-1)^{\ell'} = -(-1)^{\ell}$. From here, we can use Wigner-Eckhart theorem. For a rank-1 tensor we know that $\Delta\ell = 0, \pm 1$ and $\Delta m = 0, \pm 1$ which is consistent with our discussion above. Following from our arguments involving parity, we see that $\Delta\ell = 0$ is associated with J^0 and $\Delta\ell = \pm 1$ is associated with $\vec{J}$. We may identify a parallel to the familiar multiple radiation expansion. The electric dipole operator is, after all, $\vec{D}_E \sim \int \vec{x} J^0(\vec{x}) d^3x$, a direct connection. In general, we see the transition rules of the multiple expansion encoded in the transitions allowed by the fundamental current.

F.1.3. Matching UV to EFT

In scalar QED, the matrix element is computed from Feynman diagrams involving external bound-state wavefunctions and an insertion of $J^\mu(0)$. When approaching through an EFT, we will reproduce these matrix elements using local operators build from “effective hydrogenic fields" in an interaction term, like this:

$$\mathcal{L}_{\text{EFT}} \supset \Psi^\dagger_{n\ell m}(x) \mathcal{O}^\mu_{\text{EFT}} \Psi_{n'\ell' m'}(x) A_\mu(x) \tag{F.2}$$

By including this term in our EFT Lagrangian, we allow the dynamics of the system to include a description of transitions between states of different energy and angular momentum quantum numbers. The operator $\mathcal{O}^\mu_{\text{EFT}}$ is contracted with the vector potential $A_\mu(x)$, and as such it's components should be related to the structure of the vector potential. Further, the entire construction should match $\langle n'\ell' m' | \, J^\mu(0) \, | n\ell m \rangle$, and so should follow the same symmetries and permit the same transitions. Note that Transitions in n are handled by how much energy is absorbed or emitted.

This above is why the matrix element is sensitive to both internal structure (the wavefunction and it's angular momentum quantum numbers) and external probes (the energy of a photon absorbed/emitted by the system). Starting from the ground state transitions

$\langle n'00| J^\mu(0) |n00\rangle$ to higher states, we could build up a set of operators $\mathcal{O}^\mu_{\mathrm{EFT}}$ which correctly match the behavior of the matrix elements and systematically construct all possible forms of $\mathcal{O}^\mu_{\mathrm{EFT}}$.

F.1.4. Power Counting and EFT expansion

Consider a photon emitted during a transition with energy ω. In a non-relativistic bound state, the particles have typical velocities v. α governs coupling between the particles and the electromagnetic field, which is to say that as α increases coupling too increases, and the emitted photon will be at a higher w for a smaller relative change in v. For systems with higher constituent mass m there will be less change in velocity for a photon emitted at a given ω. Since both parameters both scale inversely (i.e. as $1/\alpha$, $1/\alpha^2$, etc.) , we can use higher powers as indicators of less relatively important contributions in the expansion.

F.2. Computing the Matrix Element in Scalar QED

Now we will explicitly compute the matrix element $\langle n'\ell'm'| J^\mu(0) |n\ell m\rangle$ to leading order in the fine-structure constant α. We will work in the center of mass frame, and treat the scalar particle ϕ with charge $-e$.

F.2.1. Bound State Structure

The bound state is a superposition of two-particle states (describing one particle and one heavy source) weighted by a Schrödinger wave function

$$|n\ell m\rangle = \int \frac{d^3\vec{p}}{(2\pi)^3} \tilde{\psi}_{n\ell m}(\vec{p}) a^\dagger_{\vec{p}} b^\dagger_{-\vec{p}} |0\rangle \,. \tag{F.3}$$

In this expression, the $a^\dagger_{\vec{p}} b^\dagger_{-\vec{p}} |0\rangle$ term uses $a^\dagger_{\vec{p}}$ to create the static, heavy charged scalar, and $b^\dagger_{-\vec{p}}$ to generate the lightweight scalar. In this context, we can take $b^\dagger_{-\vec{p}}$ to represent the static source's state implicitly. The $\tilde{\psi}_{n\ell m}(\vec{p})$ term is the hydrogenic wave function in momentum space, which satisfies the Schrödinger equation with a Coulomb potential $V(r) = -Z\frac{e^2}{4\pi r} = -Z\frac{\alpha}{r}$, where we take $Z = 1$. Angular momentum dependence is encoded within spherical harmonics, like in position space. At small $|\vec{p}|$, the dependence goes like $\propto p^\ell$, and asymptotically approaches $\sim p^{-4}$. For states close to the ground state in energy, we take this Fock-space representation to be a valid approximation since it will capture the non-relativistic behavior of the system at low energies.

F.2.2. Leading Contribution to $\langle n'\ell'm'| J^\mu(0) |n\ell m\rangle$

The scalar QED current for a complex scalar field with charge $-e$ is written as

$$J^\mu(x) = ie[\phi^\dagger(x)(\partial^\mu\phi(x)) - (\partial^\mu\phi^\dagger(x))\phi(x)] \tag{F.4}$$

where, in the non-relativistic limit,

$$\phi(x) \approx \int \frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}} a_{\vec{p}} e^{-ip\cdot x} \quad , \qquad \text{with} \quad E_p \approx m + \frac{\vec{p}^2}{2m} \tag{F.5}$$

Using the Fock-space expression for the bound states and the nonrelativistic field expansion, Eqs. (F.3) and (F.5), we will perform the wick contractions to evaluate $\langle n'\ell'm'| J^\mu(0) |n\ell m\rangle$. First, we are able to write:

$$\left\langle n'\ell'm'\right| J^\mu(0) |n\ell m\rangle = ie[\left\langle n'\ell'm'\right| \phi^\dagger(0)(\partial^\mu\phi(0)) |n\ell m\rangle - \left\langle n'\ell'm'\right| (\partial^\mu\phi^\dagger(0))\phi(0) |n\ell m\rangle]$$

We then apply

$$\begin{aligned}
\phi(x) &\approx \int \frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}} a_{\vec{p}} e^{-ip^\mu x_\mu} \rightarrow \partial^\mu\phi(x) \approx -i\int \frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}} a_{\vec{p}} e^{-ip\cdot x}(p^\mu) \\
\phi^\dagger(x) &\approx \int \frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}} a^\dagger_{\vec{p}} e^{ip^\mu x_\mu} \rightarrow \partial^\mu\phi^\dagger(x) \approx i\int \frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}} a^\dagger_{\vec{p}} e^{ip^\mu x_\mu}(p^\mu)
\end{aligned} \tag{F.6}$$

in order to identify

$$\phi^\dagger(0)(\partial^\mu\phi(0)) \approx -i\int\frac{d^3\vec{k}}{(2\pi)^3\sqrt{2E_k}}a^\dagger_{\vec{k}}\int\frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}}a_{\vec{p}}(p^\mu)$$
$$= -i(a^\dagger_{\vec{k}}a_{\vec{p}})\int\frac{d^3\vec{k}}{(2\pi)^3\sqrt{2E_k}}\frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}}(p^\mu) \tag{F.7}$$

and

$$(\partial^\mu\phi^\dagger(0))\phi(0) \approx i\int\frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}}a^\dagger_{\vec{p}}(p^\mu)\int\frac{d^3\vec{k}}{(2\pi)^3\sqrt{2E_k}}a_{\vec{k}}$$
$$= i(a^\dagger_{\vec{k}}a_{\vec{p}})\int\frac{d^3\vec{k}}{(2\pi)^3\sqrt{2E_k}}\frac{d^3\vec{p}}{(2\pi)^3\sqrt{2E_p}}(p^\mu). \tag{F.8}$$

From here, we are ready to apply the Wick contractions to identify a result. Looking to the first term,

$$\langle n'\ell'm'|\, a^\dagger_{\vec{k}}a_{\vec{p}}\,|n\ell m\rangle = \int\int\frac{d^3\vec{p''}}{(2\pi)^3}\frac{d^3\vec{p'}}{(2\pi)^3}\tilde{\psi}^*_{n'\ell'm'}(\vec{p'})\tilde{\psi}_{n\ell m}(\vec{p''})\,\langle 0|\, a_{\vec{p'}}b_{-\vec{p'}}a^\dagger_{\vec{k}}a_{\vec{p}}a^\dagger_{\vec{p''}}b^\dagger_{-\vec{p''}}\,|0\rangle \tag{F.9}$$

To interpret $\langle 0|\, a_{\vec{p'}}b_{-\vec{p'}}a^\dagger_{\vec{k}}a_{\vec{p}}a^\dagger_{\vec{p''}}b^\dagger_{-\vec{p''}}\,|0\rangle$, we can use Wick's theorem along with the commutation relation

$$a^\dagger_{\vec{k}}a_{\vec{p}} = [a^\dagger_{\vec{k}}, a_{\vec{p}}] = -(2\pi)^3\delta^3(\vec{p}-\vec{k}) \tag{F.10}$$

in order to identify the following contractions,

$$a_{\vec{p'}}a^\dagger_{\vec{k}} = (2\pi)^3\delta^3(\vec{p'}-\vec{k})$$
$$b_{-\vec{p'}}b^\dagger_{-\vec{p''}} = (2\pi)^3\delta^3(\vec{p''}-\vec{p'})$$
$$a_{\vec{p}}a^\dagger_{\vec{p''}} = (2\pi)^3\delta^3(\vec{p}-\vec{p''}) \tag{F.11}$$

which we can apply, leveraging that creation and annihilation operators a_i and $a_i^\dagger$ each commute with both b_i and $b_i^\dagger$.

$$\langle n'\ell'm'|\, \phi^\dagger(0)(\partial^\mu\phi(0))\,|n\ell m\rangle = \int \frac{d^3\vec{p}}{(2\pi)^3}\tilde{\psi}^*_{n'\ell'm'}(\vec{p})\tilde{\psi}_{n\ell m}(\vec{p})\frac{(-i)p^\mu}{2E_p}$$
$$\langle n'\ell'm'|\, (\partial^\mu\phi^\dagger(0))\phi(0)\,|n\ell m\rangle = \int \frac{d^3\vec{p}}{(2\pi)^3}\tilde{\psi}^*_{n'\ell'm'}(\vec{p})\tilde{\psi}_{n\ell m}(\vec{p})\frac{(i)p^\mu}{2E_p} \tag{F.12}$$

Combining these terms, we are able to conveniently solve Equation (F.6)

$$\langle n'\ell'm'|\, J^\mu(0)\,|n\ell m\rangle = e\int \frac{d^3\vec{p}}{(2\pi)^3}\tilde{\psi}^*_{n'\ell'm'}(\vec{p})\tilde{\psi}_{n\ell m}(\vec{p})\frac{p^\mu}{E_p} \tag{F.13}$$

In the nonrelativistic limit $p^0 \approx m$, and so to leading order

$$\langle n'\ell'm'|\, J^\mu(0)\,|n\ell m\rangle \approx \frac{e}{m}\int \frac{d^3\vec{p}}{(2\pi)^3}\tilde{\psi}^*_{n'\ell'm'}(\vec{p})p^\mu\tilde{\psi}_{n\ell m}(\vec{p}). \tag{F.14}$$

Using the Fourier transform property for spatial components,

$$\int \frac{d^3\vec{p}}{(2\pi)^3}\vec{p}\,\widetilde{\psi}(\vec{p})e^{-i\vec{p}\cdot\vec{r}} = -i\vec{\nabla}\psi(\vec{r}) \tag{F.15}$$

we can transform the momentum-space result we identified above into position space. We'll apply this identity to the un-starred wave function, and bring the conjugated wave function into position space using the typical Fourier transform,

$$\tilde{\psi}^*_{n'\ell'm'}(\vec{p}) = \int d^3\vec{r}\,\psi^*_{n'\ell'm'}(\vec{r})e^{i\vec{r}\cdot\vec{p}} \tag{F.16}$$

which introduces the exponential term needed for expression F.15. When this is done, we find that, in position space,

$$\langle n'\ell'm'|\, J^i(0)\,|n\ell m\rangle \approx \frac{-i\,e}{m}\int d^3\vec{r}\ \psi^*_{n'\ell'm'}(\vec{r})\partial^i\psi_{n\ell m}(\vec{r}) \tag{F.17}$$

The symmetrized derivative is defined as $f^*\overleftrightarrow{\partial^i}g := f^*(\partial^i g) - (\partial^i f^*)g$. To write our answer in position space in terms of this, notice that the integrand can be written like so:

$$\psi^*_{n'\ell'm'}(\partial^i\psi_{n\ell m}) = \frac{1}{2}\left(\left[\psi^*_{n'\ell'm'}(\partial^i\psi_{n\ell m}) + (\partial^i\psi^*_{n'\ell'm'})\psi_{n\ell m}\right] + \left[\psi^*_{n'\ell'm'}(\partial^i\psi_{n\ell m}) - (\partial^i\psi^*_{n'\ell'm'})\psi_{n\ell m}\right]\right)$$
$$= \frac{1}{2}\left(\partial^i(\psi^*_{n'\ell'm'}\psi_{n\ell m}) + \psi^*_{n'\ell'm'}\overleftrightarrow{\partial^i}\psi_{n\ell m}\right) \tag{F.18}$$

The first term, $\partial^i(\psi^*_{n'\ell'm'}\psi_{n\ell m})$, will vanish from the integral The "why" of this is a bit subtle - by the divergence theorem the expression becomes a surface integral, which must be zero at infinity for the bound state.

Finally, we are able to fully re-write the matrix element in position space as

$$\langle n'\ell'm'\big| J^i(0) \left|n\ell m\right\rangle \approx \frac{e}{2\,i\,m}\int d^3\vec{r}\;\psi^*_{n'\ell'm'}(\vec{r})\overset{\leftrightarrow}{\partial^i}\psi_{n\ell m}(\vec{r}). \tag{F.19}$$

From this structure, and the knowledge that we are working with a vector operator, we can reinforce the selection rules we identified earlier in table **??**. We observe that the electric dipole transition E1 is dominant.

F.2.3. Evaluating a Transition Element

Now we will compute the specific matrix element for the $2p \to 1s$ transition. The wave functions are

$$\begin{aligned}\psi_{100}(\vec{r}) &= \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\\ \psi_{21m}(\vec{r}) &= \frac{1}{\sqrt{32\pi a_0^5}}\,r\,e^{-r/(2\,a_0)}Y_{1m}(\hat{r})\end{aligned} \tag{F.20}$$

where $a_0 = 1/(Zm_e\alpha)$ is the Bohr radius. In scalar QED we take $m_e = m$, the scalar mass, and assume $Z = 1$. From here, we can set up the integral:

$$\langle 100|\,J^z(0)\,|210\rangle = \frac{e}{2\,i\,m}\int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\phi\, r^2\sin(\theta)\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\left(\partial^z\frac{1}{\sqrt{32\pi a_0^5}}\,r\,e^{-r/(2\,a_0)}Y_{10}(\hat{r})\right) \tag{F.21}$$

To evaluate $\partial^z\frac{1}{\sqrt{32\pi a_0^5}}\,r\,e^{-r/(2\,a_0)}Y_{10}(\hat{r})$, we recall that $Y_{10} = \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{z}{r}$, $r = \sqrt{x^2+y^2+z^2}$. We can then rewrite

$$\partial^z\frac{1}{\sqrt{32\pi a_0^5}}\,r\,e^{-r/(2\,a_0)}Y_{10}(\hat{r}) = \partial^z\frac{z\sqrt{3}}{\pi\sqrt{128a_0^5}}\;e^{-\sqrt{x^2+y^2+z^2}/(2\,a_0)} \tag{F.22}$$

which evaluates to

$$\begin{aligned}\partial^z \frac{1}{\sqrt{32\pi a_0^5}}\, r\, e^{-r/(2\,a_0)} Y_{10}(\hat{r}) =& \frac{\sqrt{3}}{\pi\sqrt{128 a_0^5}} e^{-r/(2\,a_0)} + \frac{\sqrt{3}}{2\pi\, a_0 \sqrt{128 a_0^5}}\, \frac{z^2}{r}\, e^{-r/(2\,a_0)} \\ =& \frac{\sqrt{3}}{\pi\sqrt{128 a_0^5}} e^{-r/(2\,a_0)} \left(1 + \frac{1}{2a_0}\frac{z^2}{r}\right) \\ =& \frac{\sqrt{3}}{\pi\sqrt{128 a_0^5}} e^{-r/(2\,a_0)} \left(1 + \frac{1}{2a_0} r\cos^2(\theta)\right). \qquad \text{(F.23)}\end{aligned}$$

The integral for the matrix element is then

$$\begin{aligned}\langle 100|\, J^z(0)\, |210\rangle =& \frac{e}{2\,i\,m}\int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi\, r^2 \sin(\theta)\, \frac{\sqrt{3}}{a_0^4\sqrt{128\pi^3}} \left(1 + \frac{1}{2a_0} r\cos^2(\theta)\right) e^{-(3\,r)/(2\,a_0)} \\ =& \frac{e}{2\,i\,m}\frac{\sqrt{3}}{a_0^4\sqrt{128\pi^3}} \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\phi \left[\left(r^2 \sin(\theta)\, e^{-(3\,r)/(2\,a_0)}\right) + \frac{1}{2a_0}\left(r^3 \sin(\theta)\cos^2(\theta)\, e^{-(3\,r)/(2\,a_0)}\right)\right]\end{aligned}$$

Integrating this, we find that this particular element evaluates to

$$\langle 100|\, J^z(0)\, |210\rangle = \frac{4\,e}{27\,i\,a_0\,m}\sqrt{\frac{2}{3\pi}} = \frac{4\,e\,\alpha}{27\,i}\sqrt{\frac{2}{3\pi}}. \qquad \text{(F.24)}$$

Looking at the scaling of this result, we observe that

$$\begin{aligned}\langle 100|\, J^z(0)\, |210\rangle &\propto e \\ &\propto \alpha \\ &\propto 1/a_0\end{aligned}$$

as expected.

F.3. Matching to the Effective Theory of Hydrogenic Fields

Now that we have both explored the general structure of the matrix element and carried out an explicit calculation for an example transition, we will now return to our discussion of EFTs. In this section, we will reproduce the matrix element $\langle n'\ell'm'|\, J^\mu(0)\, |n\ell m\rangle$ using local EFT operations for bound state dynamics.

F.3.1. Constructing the Operator

We'll consider an EFT interaction term, responsible for coupling to the electromagnetic current (or an external photon A_μ):

$$\mathcal{L}_{\mathrm{EFT}} \supset \Psi^\dagger_{n'\ell'm'}(c^\mu \mathcal{O}_{\mathrm{base}})\Psi_{n\ell m}. \tag{F.25}$$

c^μ is a Wilson coefficient, and $\mathcal{O}_{\mathrm{base}}$ is a simple operator structure. From a symmetry perspective, the form of $\mathcal{O}_{\mathrm{base}}$ is restricted by the fact that it couples the states to the spatial part of the current J^i and so should follow the same symmetry. That is, $\mathcal{O}_{\mathrm{base}}$ should be odd under parity and charge conjugation, and should be Hermitian.

F.3.2. Considering an Emitted Photon

Consider a photon emitted with energy $\omega \sim m\alpha^2 Z$ and an internal velocity $v \sim \alpha Z$. The matrix element of a leading EFT operator should scale in $m, \alpha,$ and Z in the same way as the matrix element of J^i. Higher-order operations would be suppressed in this expansion via power counting.

F.3.3. Matching to Fix the Wilson Coefficient

The goal is to match the UV theory result,

$$\langle n'\ell'm'|\, J^i(0)\, |n\ell m\rangle \approx \frac{-i\, e}{m_\phi} \int d^3\vec{r}\ \psi^*_{n'\ell'm'}(\vec{r})\partial^i \psi_{n\ell m}(\vec{r}) \tag{F.26}$$

to the EFT. Choosing a simple base operator structure, related to $\Psi^\dagger$(derivative)Ψ, we can define a suitable leading-order EFT operator that reproduces the structure of $J^i_{\rm QED}$ simply:

$$\mathcal{O}^i_{\rm EFT} = -\frac{i\,e}{m_\phi}\partial^i \tag{F.27}$$

what about the differences between $|\Psi_{n\ell m}\rangle$ and $|n\ell m\rangle$? They're not "literally" the same thing, since $|n\ell m\rangle$ are genuinely the hydrogenic bound states and $|\Psi_{n\ell m}\rangle$ are the states of the quantum field in our EFT, but they describe the same physics.

Here we can see how the EFT "knows" about the underlying physics. This direct connection is manifest in both the matching of the first order behavior of J^i's matrix element and in the direct dependence on physical quantities relevant to the problem, being the mass and the charge.

F.4. Toward Non-Abelian and Gravitational Bound States

We can use this case study as a primer for a later investigation into gravitational systems, though there will be some key differences. Scalar QED is a relatively simple construction compared to Yang-Mills theory and gravity where the force mediators can (and do) self-interact. When we go on to discuss YM and gravity, we will need to account for this new behavior and will be able to use it to identify "new corrections" in the classical limit.

F.5. UV to EFT: Takeaways

In this section, we computed a matrix element of the electromagnetic current between bound states in scalar QED and matched this result to an EFT.

We've observed that relativistic QFT (for us, scalar QED) contains the non-relativistic Schrödinger atom description as a consistent limit. This is a significant feature of a quantum field theory - indeed, we should be able to recover familiar non-relativistic results by taking limits just as we are able to recreate classical results in the limits of non-relativistic quantum mechanics.

To accomplish this relation, however, we did make some key assumptions. We assumed that one scalar particle was so much more massive than the other that it could be treated as non-recoiling, and that bound states were entirely made up of particles (no antiparticles).

As we move to more complex scenarios like QCD bound states and gravitational systems, this overall strategy will work as a framework we will see challenges in several areas. Since gluons and gravitons can self interact, the loop structure at leading order will be more complicated and thus the QFT calculation naturally would become more difficult. There will also be more topologies to consider, with different amounts of internal massive and gluon (or graviton) propagators.