Tutorial on translating particle physics effective Lagrangians to conventional atomic physics and quantum chemistry operators

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May 31, 2013

Occasionally we have to carry out calculations with some effective Lagrangians supplied by our particle physics friends (possibly related to new physics beyond the standard model). For example, we could be given a Lagrangian density

$$\mathcal{L}' = g\ \phi\bar{\psi}\psi\,,$$

where ϕ is some scalar field, ψ is the Dirac field (electrons) and g is a coupling constant. The Dirac equation that is conventionally used in atomic physics reads

$$\begin{aligned} H_D &= c\alpha\cdot\mathbf{p}+\beta m_e c^2+V'\,, \\ i\hbar\frac{\partial}{\partial t}\psi &= H_D\psi\,. \end{aligned} \tag{1}$$

(Here and below I suppress interactions of electrons with each other and with the nucleus). Given $\mathcal{L}'$ what is that extra operator V' that I would have to add to my Dirac Hamiltonian? The answer depends on particle physics conventions and I will consistently derive V' below.

First of all, since in classical mechanics $L = T - V$, it is tempting to write $V' = -\mathcal{L}'$, which is certainly incorrect. So let's track what happens to $\mathcal{L}'$ as I derive Eq.(1) from the lagrangian formulation. For the impatient, the result is

$$V'\psi = -\gamma_0\left(\frac{\partial\mathcal{L}'}{\partial\bar{\psi}}-\partial_\mu\left(\frac{\partial\mathcal{L}'}{\partial\left(\partial_\mu\bar{\psi}\right)}\right)\right). \tag{2}$$

We start by writing out the total Lagrangian density

$$\mathcal{L} = \mathcal{L}_D+\mathcal{L}_\phi+\mathcal{L}'. \tag{3}$$

Here $\mathcal{L}_D$ and $\mathcal{L}_\phi$ are Lagrangians for uncoupled fields.

$$\mathcal{L}_D = i\left(\hbar c\right)\bar{\psi}\gamma^\mu\partial_\mu\psi-\left(m_e c^2\right)\bar{\psi}\psi \tag{4}$$

is the Dirac (spin 1/2) Lagrangian that I would need and I am going to keep $\mathcal{L}_\phi$ unspecified. I use the Bjorken and Drell conventions for the Dirac matrices γ.

The field equations are derived from the Eurler-Lagrange formula

$$\partial_\mu \left(\frac{\partial \mathcal{L}}{\partial \left(\partial_\mu \Phi \right)} \right) = \frac{\partial \mathcal{L}}{\partial \Phi}, \tag{5}$$

where Φ spans all quantum fields in the problem. Since the Dirac field ψ is complex valued, I can treat ψ and $\bar{\psi}$ as independent quantities.

The Eurler-Lagrange formula applied to the Dirac Lagrangian yields

$$\frac{\partial \mathcal{L}_D}{\partial \bar{\psi}} = i \left(\hbar c \right) \gamma^\mu \partial_\mu \psi - \left(m_e c^2 \right) \psi, \tag{6}$$

$$\frac{\partial \mathcal{L}_D}{\partial \left(\partial_\mu \bar{\psi} \right)} = 0. \tag{7}$$

Then the free-particle Dirac equation with extra juice coming from the $\mathcal{L}'$ contribution

$$i \left(\hbar c \right) \gamma^\mu \partial_\mu \psi - \left(m_e c^2 \right) \psi + \left(\frac{\partial \mathcal{L}'}{\partial \bar{\psi}} - \partial_\mu \left(\frac{\partial \mathcal{L}'}{\partial \left(\partial_\mu \bar{\psi} \right)} \right) \right) = 0. \tag{8}$$

Notice that this differs from Eq.(1) used in atomic physics and quantum chemistry. For example, the rest-energy term does not contain β and we need to add an extra step: since $\beta = \gamma_0$, I multiply through with γ_0 (I will only keep the first term for $\mathcal{L}'$ and recover the second term later on).

$$\gamma_0 \frac{\partial \mathcal{L}}{\partial \bar{\psi}} = i \left(\hbar c \right) \gamma_0 \gamma^\mu \partial_\mu \psi - \gamma_0 \left(m_e c^2 \right) \psi + \gamma_0 \frac{\partial \mathcal{L}'}{\partial \bar{\psi}} = 0 \tag{9}$$

$$\gamma_0 \gamma^\mu \partial_\mu \psi = \gamma_0 \gamma^0 \partial_0 \psi + \gamma_0 \gamma^i \partial_i \psi = \tag{10}$$

$$= \left(\gamma^0 \right)^2 \partial_0 \psi + \gamma_0 \gamma^i \partial_i \psi = \left(\gamma^0 \right)^2 \frac{1}{c} \frac{\partial}{\partial t} \psi + \gamma_0 \gamma^i \frac{\partial}{\partial x^i} \psi \tag{11}$$

$$\left(\gamma^0 \right)^2 = 1$$

$$\gamma_0 \gamma^i = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = \alpha^i \tag{12}$$

The matrices α^i are the same as the ones in Eq.(1). Then, since $i\hbar \frac{\partial}{\partial x^i} = p_i$

$$i \left(\hbar c \right) \gamma_0 \gamma^i \frac{\partial}{\partial x^i} \psi = c \sum_i \alpha^i \left(i\hbar \frac{\partial}{\partial x^i} \right) = c \sum_i \alpha^i p_i = -c \ \left(\alpha \cdot \mathbf{p} \right). \tag{13}$$

Finally,

$$0 = i \left(\hbar c \right) \gamma_0 \gamma^\mu \partial_\mu \psi - \gamma_0 \left(m_e c^2 \right) \psi + \gamma_0 \frac{\partial \mathcal{L}'}{\partial \bar{\psi}} =$$

$$= i\hbar \frac{\partial}{\partial t} \psi - c\alpha \cdot \mathbf{p} \psi - \beta \left(m_e c^2 \right) \psi + \gamma_0 \frac{\partial \mathcal{L}'}{\partial \bar{\psi}}$$

Or

$$i\hbar\frac{\partial}{\partial t}\psi = c\alpha\cdot\mathbf{p}\psi + \beta\left(m_e c^2\right)\psi - \gamma_0\frac{\partial\mathcal{L}'}{\partial\bar{\psi}}$$

i.e., we indeed recover Eq.(1).

Now we can easily identify that extra term in the Dirac Hamiltonian due to $\mathcal{L}'$,

$$V'\psi = -\gamma_0\left(\frac{\partial\mathcal{L}'}{\partial\bar{\psi}} - \partial_\mu\left(\frac{\partial\mathcal{L}'}{\partial\left(\partial_\mu\bar{\psi}\right)}\right)\right). \tag{14}$$

Let's consider several examples.

1 Examples

1.1 Coupling to electromagnetic fields

$$\mathcal{L}' = -\frac{1}{c}J^\mu A_\mu = -q\bar{\psi}\gamma^\mu\psi A_\mu\,, \tag{15}$$

where A is the four-vector potential $A^\mu = (\phi, \mathbf{A})$ and J is the conventional electromagnetic current density,$J^\mu = cq\bar{\psi}\gamma^\mu\psi$.

From Eq.(14)

$$V'\psi = -\gamma_0\left(\frac{\partial}{\partial\bar{\psi}}\left(-q\bar{\psi}\gamma^\mu\psi A_\mu\right) - 0\right) = q\gamma_0\gamma^\mu A_\mu\psi,$$

or

$$V' = q\gamma_0\gamma^\mu A_\mu\,.$$

Explicitly,

$$V' = q\gamma_0\gamma^0\phi + q\gamma_0\gamma^i A_i = q\phi - q\left(\alpha\cdot\mathbf{A}\right)$$

which is, of course, the familiar coupling to EM fields.

1.2 "Higgs portal"

$$\mathcal{L}' = g\ \phi\bar{\psi}\psi \tag{16}$$

$$V' = -g\phi\gamma_0 = -g\phi\beta \tag{17}$$

Compare $\mathcal{L}'$ to the rest-energy term in the Dirac Lagrangian, $-m_e c^2\bar{\psi}\psi$. V' has the same structure as the rest mass term in the Dirac Hamiltonian, as it should. Effecttively the mass of the electron is modified

$$m_{\text{eff}}c^2 = m_e c^2 - g\phi$$

1.3 Axion fields

Here are two equivalent expressions for the Lagrangian describing coupling of pseudoscalar axions to electrons

$$\mathcal{L}' = 2\frac{m_e}{f_a} a \ \overline{\psi} i \gamma_5 \psi, \tag{18}$$

$$\mathcal{L}'' = -\frac{1}{f_a} \left(\partial_\mu a\right) \ \overline{\psi} \gamma^\mu \gamma_5 \psi. \tag{19}$$

Here a is the axion field and f_a is a coupling constant.

Then

$$V' = -2\frac{m_e}{f_a} a \ i\gamma_0\gamma_5$$
$$V'' = \frac{1}{f_a} \left(\partial_\mu a\right) \ \gamma_0 \gamma^\mu \gamma_5.$$

Explicitly V''

$$V'' = \frac{1}{f_a} \left(\partial_0 a\right) \ \gamma_0 \gamma^0 \gamma_5 + \frac{1}{f_a} \left(\partial_i a\right) \ \gamma_0 \gamma^i \gamma_5 =$$
$$\frac{1}{c f_a} \left(\frac{\partial a}{\partial t}\right) \gamma_5 + \frac{1}{f_a} \sum_i \frac{\partial a}{\partial x^i} \Sigma^i,$$

where

$$\Sigma^i = \gamma_0 \gamma^i \gamma_5 = \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}.$$