1 Lagrangian and Hamiltonian for the Dirac equation

Like in classical mechanics, one can use a Lagrangian $L = \int \mathrm{d}^3x\, \mathcal{L}$ (where $\mathcal{L}$ is the Lagrangian density) also in classical field theory: The field equations (Euler Lagrange equations) should follow from the invariance of the action $S = \int \mathrm{d}t\, L = \int \mathrm{d}^4x\, \mathcal{L}$ under an arbitrary variation of the fields and their derivatives. This assumption is called the variational principle: $\delta S = 0$. The Hamiltonian is then obtained from the Lagrangian by a Legendre transformation. In this Section, we derive the Lagrangian and the Hamiltonian for the Dirac equation.

The Dirac equations for $\psi(x)$ and $\overline{\psi}(x) = \psi^\dagger(x)\gamma^0$ are (see Sect. 5 of RQM1)

$$(i\partial\!\!\!/ - m)\,\psi(x) = 0\,, \qquad \overline{\psi}(x)\left(-i\overleftarrow{\partial\!\!\!/} - m\right) = 0 \tag{1.1}$$

They can be derived form the following Lagrangian density:

$$\mathcal{L} = \overline{\psi}(x)\,(i\partial\!\!\!/ - m)\,\psi(x) = \overline{\psi}\,(i\gamma^\mu\partial_\mu - m)\,\psi \tag{1.2}$$

Show this: The action, as a functional of the independent fields ψ and $\overline{\psi}$ and their derivatives, is:

$$S = \int \mathrm{d}^4x\, \mathcal{L}\left(\psi, \partial_\mu\psi; \overline{\psi}, \partial_\mu\overline{\psi}\right) \tag{1.3}$$

Under arbitrary (infinitesimal) variation of the fields ψ, $\overline{\psi}$ and their derivatives, the variation of the action is then

$$\delta S = \int \mathrm{d}^4x\, \delta\mathcal{L} = \int \mathrm{d}^4x \left[\frac{\partial\mathcal{L}}{\partial\psi}\,\delta\psi + \frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\psi\right)}\,\delta\left(\partial_\mu\psi\right) + \frac{\partial\mathcal{L}}{\partial\overline{\psi}}\,\delta\overline{\psi} + \frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\overline{\psi}\right)}\,\delta\left(\partial_\mu\overline{\psi}\right)\right] \tag{1.4}$$

Using $\delta\left(\partial_\mu\psi\right) = \partial_\mu\left(\delta\psi\right)$ in the second term, and $\delta\left(\partial_\mu\overline{\psi}\right) = \partial_\mu\left(\delta\overline{\psi}\right)$ in the fourth term, and performing partial integrations, we get

$$\delta S = \int \mathrm{d}^4x \left[\left(\frac{\partial\mathcal{L}}{\partial\psi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\psi\right)}\right)\delta\psi + \left(\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\overline{\psi}\right)}\right)\delta\overline{\psi}\right]$$

Because the variational principle $\delta S = 0$ must hold for arbitrary variations $\delta\psi$ and $\delta\overline{\psi}$, we obtain the "Euler-Lagrange equations"

$$\left(\frac{\partial\mathcal{L}}{\partial\psi} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\psi\right)}\right) = 0\,, \qquad \left(\frac{\partial\mathcal{L}}{\partial\overline{\psi}} - \partial_\mu\frac{\partial\mathcal{L}}{\partial\left(\partial_\mu\overline{\psi}\right)}\right) = 0 \tag{1.5}$$

Inserting here the Lagrangian density (1.2), the equations (1.5) are identical to the Dirac equations (1.1).

Note that the Lagrangian (1.2) is a scalar under Lorentz transformations and parity transformations.

In the Hamiltonian formulation, one uses the "canonical momenta"

$$\Pi_\psi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\psi^\dagger \,, \qquad \Pi_{\psi^\dagger} = \frac{\partial \mathcal{L}}{\partial \dot{\psi}^\dagger} = 0$$

instead of the time derivatives $\dot{\psi}$ and $\dot{\psi}^\dagger$. The Legendre transformation from the Lagrangian to the Hamiltonian is then given by

$$\begin{aligned}\mathcal{H} &= \Pi_\psi\, \dot{\psi} + \Pi_{\psi^\dagger}\, \dot{\psi}^\dagger - \mathcal{L} = i\psi^\dagger\, \dot{\psi} - i\psi^\dagger\, \dot{\psi} - \overline{\psi}\left(i\gamma^i\,\partial_i - m\right)\psi \\ &= \psi^\dagger\left(i\gamma^0\vec{\gamma}\cdot\vec{\nabla} + \gamma^0 m\right)\psi = \psi^\dagger\left(\vec{\alpha}\cdot\hat{\vec{p}} + \beta m\right)\psi = \psi^\dagger\, H\,\psi \end{aligned} \tag{1.6}$$

where $H = \vec{\alpha}\cdot\hat{\vec{p}} + \beta m$ is the usual Dirac Hamiltonian. If we insert here our positive and negative energy solutions (see Sect. 5 of RQM1)

$$\begin{aligned}\psi^{(+)}(\vec{x},t) &= \frac{1}{\sqrt{V}}\sqrt{\frac{m}{E_p}}\, u(\vec{p},s) e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar} \\ \psi^{(-)}(\vec{x},t) &= \frac{1}{\sqrt{V}}\sqrt{\frac{m}{E_p}}\, v(-\vec{p},s) e^{i(E_p t + \vec{p}\cdot\vec{x})/\hbar}\end{aligned}$$

we get the obvious results $\mathcal{H} = E_p/V$ for the positive energy case, and $\mathcal{H} = -E_p/V$ for the negative energy case.

The form of the Lagrangian density including an external electromagnetic field $A^\mu = \left(\phi, \vec{A}\right)$ is obtained by making the "minimal substitution" (see Sect. 10 of RQM1) in the Dirac Lagrangian (1.2):

$$\mathcal{L} = \overline{\psi}\left(i\partial\!\!\!/ - m - qA\!\!\!/\right)\psi = \mathcal{L}_0 - q\left(\overline{\psi}\gamma_\mu\psi\right)\, A^\mu \tag{1.7}$$

The Euler-Lagrange equations (1.5) then give the Dirac equations in an external field (see Sect. 10 of RQM1). The interaction part of the Lagrangian density (1.7) has the characteristic form $\mathcal{L}_I = -qj_\mu\, A^\mu$, where q is the electric charge and $j_\mu = \overline{\psi}\gamma_\mu\psi$ is the conserved current.

Following this example, one can "guess" the interaction Lagrangians for other types of interactions (strong, weak). For example, in the case of an external pion field ($\pi(x)$), a possible form of the interaction Lagrangian is [1]:

$$\mathcal{L}_I = -ig\,\left(\overline{\psi}\gamma_5\psi\right)\,\pi(x) \tag{1.8}$$

[1]The spin 1/2 field in Eq.(1.8) is a nucleon field or quark field.

Reason: Because the pion has negative parity ($\pi(-\vec{x},t) = \pi(\vec{x},t)$), it must couple to the pseudo-scalar "current" $\overline{\psi}\gamma_5\psi$ (see Sect. 7 of RQM1), so that the Lagrangian is a scalar. (The factor i is necessary for hermiticity.) The constant g is called a coupling constant. The interaction (1.8) is called a "pseudo-scalar interaction". It plays an important role in the Yukawa theory of nuclear forces.

However, there is also another possible interaction Lagrangian of the form

$$\mathcal{L}_I = g' \left(\overline{\psi}\gamma_5\gamma_\mu\psi\right) \left(\partial^\mu \pi(x)\right) \tag{1.9}$$

Here $\overline{\psi}\gamma_5\gamma_\mu\psi$ is a pseudo-vector (see Sect. 7 of RQM1), and $\partial^\mu\pi(x)$ is also a pseudo-vector, therefore (1.9) is a scalar. This form is called a "pseudo-vector interaction". In the general case, the interaction Lagrangian for pions and nucleons (or quarks) is a sum of both terms (1.8) and (1.9).

2 Klein-Gordon equation

Klein-Gordon (K.G.) equation is a relativistic wave equation for spin zero particles. $\Rightarrow$ The wave function has only 1 component: $\psi(x)$, which must be Lorentz invariant: $\psi'(x') = \psi(x)$, where $x' = \Lambda\, x$.

To get such a wave equation, we square the Dirac equation: From Sect. 3 of RQM1, the Dirac Hamiltonian is $H = (\vec{\alpha}\cdot\hat{\vec{p}})c + \beta\, mc^2$, and the matrices $\vec{\alpha}$, β were constructed such that $H^2 = -\hbar^2 c^2\,\Delta + m^2c^4$. Therefore, squaring the Dirac equation gives

$$\begin{aligned} i\hbar\dot{\psi} &= H\,\psi \Rightarrow -\hbar^2\ddot{\psi} = H^2\,\psi = \left(-\hbar^2c^2\,\Delta + m^2c^4\right)\psi \\ &\Rightarrow \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2} - \Delta\psi + \left(\frac{mc}{\hbar}\right)^2\psi = 0 \end{aligned}$$

This give the K.G. equation in the form

$$\left(\Box + \left(\frac{mc}{\hbar}\right)^2\right)\psi(x) = 0 \tag{2.1}$$

where the d'Alembert operator is defined by (see Sect. 1 of RQM1) $\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta$. Plane wave solutions of (2.1) are of the form

$$\psi_{\vec{p}}(\vec{x},t) = N\, e^{-i(Et - \vec{p}\cdot\vec{x})/\hbar} \tag{2.2}$$

They are eigenfunctions of the momentum operator $\hat{\vec{p}} = -i\hbar\vec{\nabla}$ with eigenvalue $\vec{p}$, and $N(p)$ is a normalization constant. In order that (2.2) is a solution of (2.1), E must have the form

$$E^2 = \vec{p}^2 c^2 + (mc^2)^2 \Rightarrow E = \pm\sqrt{\vec{p}^2 c^2 + (mc^2)^2} \equiv \pm E_p \tag{2.3}$$

where $E_p = \sqrt{\vec{p}^2 c^2 + (mc^2)^2} > 0$.

Does Eq.(2.3) mean that the K.G. equation has negative energy solutions, like the Dirac equation? No ! For the Klein-Gordon case, E is <u>not</u> the eigenvalue of some Hamiltonian (because the K.G. equation does <u>not</u> have the form $i\hbar\dot{\psi} = H\psi$), but just the "frequency" of the solutions (2.2): $E = E_p > 0$ means <u>positive frequency</u>, and $E = -E_p < 0$ means <u>negative frequency</u>:

$$\psi_{\vec{p}}^{(+)}(\vec{x}, t) = N(p)\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar} \tag{2.4}$$

$$\psi_{\vec{p}}^{(-)}(\vec{x}, t) = N(p)\, e^{-i(-E_p t - \vec{p}\cdot\vec{x})/\hbar} \tag{2.5}$$

We will show later that for both cases the energy is <u>positive</u>.

<u>Current conservation</u>

Multiplying the K.G. equation (2.1) by ψ^*, and the c.c. of (2.1) by ψ, and taking the difference of these two equations, we obtain

$$\partial_\mu \left[\psi^* \partial^\mu \psi - \psi\, \partial^\mu \psi^*\right] = 0 \tag{2.6}$$

This has the form of current conservation: $\partial_\mu j^\mu = 0$. However, we cannot interpret j^0 as a "probability density", because it is <u>not positive definite</u>!

If we multiply the current in Eq.(2.6) by $i\hbar q$, where $q > 0$ is the electric charge of the particle, we obtain $\partial_\mu j_c^\mu = 0$, where

$$j_c^\mu = i\hbar q \left[\psi^* \partial^\mu \psi - \psi\, \partial^\mu \psi^*\right] \tag{2.7}$$

We can interpret $j_c^\mu = (c\,\rho_c, \vec{j}_c)$ as the "electric 4-vector current": The "charge density" is given by

$$\rho_c = \frac{i\hbar}{c^2} q \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t}\right) \tag{2.8}$$

If we insert the solutions (2.4) and (2.5) into (2.8), we obtain

$$\rho_c^{(+)} = \frac{i\hbar}{c^2} q \left(\frac{-2iE_p}{\hbar}\right) N(p)^2 = \frac{2E_p q}{c^2}\, N^2 \equiv \frac{q}{V}$$

$$\rho_c^{(-)} = \frac{i\hbar}{c^2} q \left(\frac{2iE_p}{\hbar}\right) N(p)^2 = -\frac{2E_p q}{c^2}\, N^2 \equiv \frac{-q}{V}$$

where we have set the normalization factor equal to

$$N(p) = \sqrt{\frac{c^2}{2E_p V}} \tag{2.9}$$

Therefore the solution (2.4) describes a particle with charge $q > 0$, and (2.5) describes the antiparticle with charge $-q < 0$. Therefore we can interpret the conserved current (2.7) as the electric current [2].

Home work: Use the "minimal substitution" (see No. 7) $\partial^\mu \to \partial^\mu + \frac{iq}{\hbar c} A^\mu$ to obtain the Klein-Gordon equation in an external electromagnetic field A^μ, and derive the current conservation for this case. Show that the conserved electric current is then given by

$$j_c^\mu = i\hbar q \left[\psi^* \partial^\mu \psi - \psi \, \partial^\mu \psi^* + \frac{2iq}{\hbar c} A^\mu \, \psi^* \, \psi \right]$$

Show that this current is invariant under the local gauge transformations given in Sect. 10 of RQM1.

Lagrangian and Hamiltonian for Klein-Gordon field

The Lagrangian density for the free Klein-Gordon field is given by

$$\frac{1}{\hbar^2} \mathcal{L} = (\partial_\mu \psi^*) \, (\partial^\mu \psi) - \left(\frac{mc}{\hbar} \right)^2 \psi^* \, \psi \tag{2.10}$$

Check this: The requirement that $\delta S = 0$ under variations of the fields ψ and ψ^* (and their derivatives) gives the Euler-Lagrange equations [3]

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} &= 0 \\ \frac{\partial \mathcal{L}}{\partial \psi^*} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi^*)} &= 0 \end{aligned}$$

Inserting here the Lagrangian density (2.10), these equations become identical to the Klein-Gordon equations (2.1) for ψ and ψ^*.

For the transformation to the Hamiltonian density, we need the "canonical momenta" of ψ and ψ^*:

$$\begin{aligned} \Pi_\psi &\equiv \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \frac{\hbar^2}{c^2} \dot{\psi}^* \equiv \Pi \\ \Pi_{\psi^*} &\equiv \frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = \frac{\hbar^2}{c^2} \dot{\psi} = \Pi^* \end{aligned}$$

[2] In order to describe also neutral particle consistently with the Klein-Gordon equation, one needs the methods of quantum field theory.

[3] The calculation is the same as for the Dirac case, with the replacement $\overline{\psi} \to \psi^*$.

Then the Hamiltonian density is given by

$$\begin{aligned}\mathcal{H} &= \Pi\,\dot{\psi} + \Pi^*\,\dot{\psi}^* - \mathcal{L} = 2\left(\frac{c^2}{\hbar^2}\right)\Pi\,\Pi^* - \left(\frac{c^2}{\hbar^2}\right)\Pi\,\Pi^* + \hbar^2\left(\vec{\nabla}\psi^*\right)\cdot\left(\vec{\nabla}\psi\right) + (mc)^2\;\psi^*\,\psi \\ &= \left(\frac{c^2}{\hbar^2}\right)|\Pi|^2 + \hbar^2|\vec{\nabla}\psi|^2 + (mc)^2\,|\psi|^2 > 0 \qquad (2.11)\end{aligned}$$

Because this is positive definite, the Hamiltonian $H = \int \mathrm{d}^3x\,\mathcal{H}$ is also positive definite. Therefore, in the classical field theory, there are no negative energies of the Klein-Gordon field!

As a check of (2.11), we can insert the solutions (2.4) and (2.5) into (2.11), using the normalization factor given by (2.9), and find

$$\mathcal{H}^{(+)} = \mathcal{H}^{(-)} = \frac{E_p}{V}$$

which is indeed the energy density (energy E_p per volume V) of a free particle.