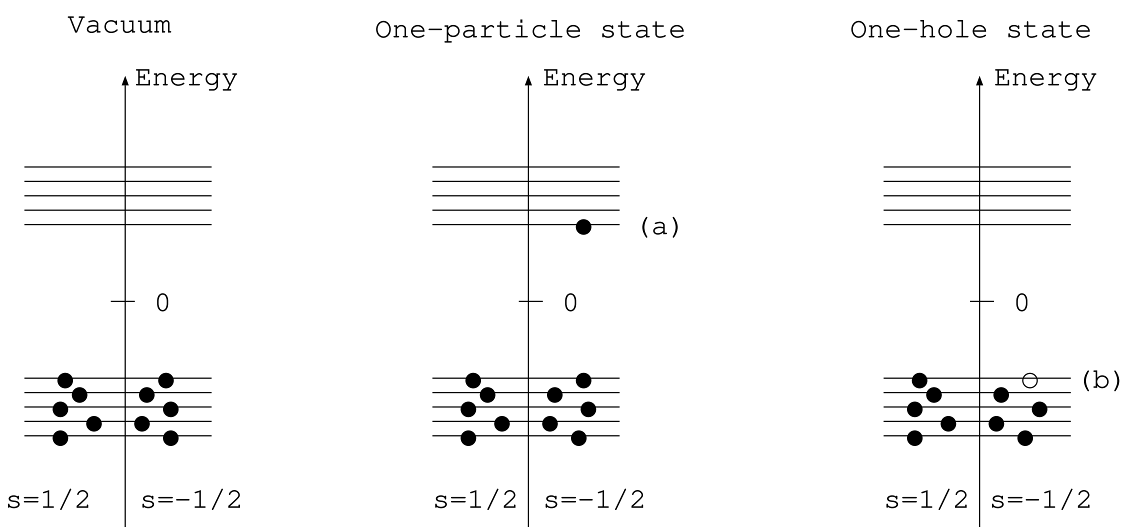
12 Dirac's hole theory

Remember: The Dirac equation is a 4×4 matrix equation, and therefore it has four independent solutions. For a free particle with momentum $\vec{p}$, we have obtained these four solutions in Sect. 4. They have the following values for the energy E and spin component s (along some axis): (i) $(E, s) = (E_p, \frac{1}{2})$, where $E_p = \sqrt{(mc^2)^2 + (\vec{p}c)^2}$; (ii) $(E, s) = (E_p, -\frac{1}{2})$; (iii) $(E, s) = (-E_p, \frac{1}{2})$; (iv) $(E, s) = (-E_p, -\frac{1}{2})$.

Problem: What is the physical meaning of the solutions with negative energy?

For simplicity, consider a finite system (a box), where the single particle energies are discrete (because of the boundary conditions). In the energy level diagram below, each line represents a single particle state $(E, \vec{p}, s)$, where $E = \pm E_p$ is the energy, $\vec{p}$ is the momentum, and $s = \pm\frac{1}{2}$ is the spin direction. Dirac defined the "vacuum state", the "one-particle state", and the "one-hole state" as follows:



1. Vacuum: All negative energy levels are filled, according to the Pauli principle. All positive energy levels are empty.

   This "vacuum state" (reference state) has:

   - energy $E = -\infty$, but by "renormalization" [1] it gets zero energy:
     $E = -\infty \overset{\text{renormalization}}{\longrightarrow} E = 0$;
   - zero momentum (because for each occupied momentum $\vec{p}$, also $-\vec{p}$ is occupied):
     $\vec{P} = \vec{0}$;

[1] By "renormalization" we mean to subtract an infinity, i.e., a new definition of "zero energy" or "zero charge".

- zero spin (because $s = 1/2$ and $s = -1/2$ are occupied):
  $S = 0$;

- charge $Q = -\infty$, but by "renormalization" is gets zero charge:
  $Q = -\infty \overset{\text{renormalization}}{\longrightarrow} Q = 0$.

This kind of vacuum state is also called the "Dirac sea".

2. One-particle state: All negative energy levels are filled. In the positive energy level (a), which has $(E = +E_p, \vec{p}, s)$, one electron is *added*.

   This "one-particle state" has:

   - energy $E = -\infty + E_p \overset{\text{renormalization}}{\longrightarrow} E = +E_p$;
   - momentum $\vec{P} = \vec{0} + \vec{p} = \vec{p}$;
   - spin $S = 0 + s = s$;
   - charge $Q = -\infty + e \overset{\text{renormalization}}{\longrightarrow} Q = e < 0$.

3. Single-hole state: All positive energy levels are empty. In the negative energy level (b), which has $(E = -E_p, -\vec{p}, -s)$, one electron is *missing*.

   This "one-hole state" has:

   - energy $E = -\infty - (-E_p) \overset{\text{renormalization}}{\longrightarrow} E = +E_p$;
   - momentum $\vec{P} = \vec{0} - (-\vec{p}) = \vec{p}$;
   - spin $S = 0 - (-s) = s$;
   - charge $Q = -\infty - e \overset{\text{renormalization}}{\longrightarrow} Q = -e > 0$.

We see: The "one-particle state" and "one-hole state" have the same energy (both positive!), momentum and spin, but opposite charge. $\Rightarrow$ One can interpret the "one-hole state" as the "antiparticle" (positron) state. In this way, Dirac predicted the positron, which differs from the electron only by the opposite charge. It was found by Anderson in 1933 in the cosmic rays.

The free Dirac wave functions, normalized in a volume V, are (see Sect. 4):

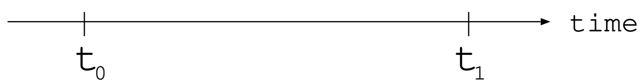
1. For electron ("one-particle state") with energy $E_p > 0$, momentum $\vec{p}$, spin s, charge $e < 0$:

$$\psi^{(+)}_{\vec{p},s}(\vec{x}, t) = \frac{1}{\sqrt{V}} \sqrt{\frac{mc^2}{E_p}}\, u(\vec{p}, s)\, e^{-i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

2. For positron ("one-hole state") with energy $E_p > 0$, momentum $\vec{p}$, spin s, charge $-e > 0$:

$$\psi^{(-)}_{-\vec{p},-s}(\vec{x},t) = \frac{1}{\sqrt{V}} \sqrt{\frac{mc^2}{E_p}}\, v(\vec{p},-s)\, e^{i(E_p t - \vec{p}\cdot\vec{x})/\hbar}$$

However, there is a problem with time evolution:



When a positron evolves from time t_0 (its "creation") to a later time $t_1 > t_0$ (its "annihilation"):

- At time $t = t_0$: Creation of positive energy positron $\equiv$ Annihilation of negative energy electron (= making a hole in the Dirac sea).
- At time $t = t_1$: Annihilation of positive energy positron $\equiv$ Creation of negative energy electron (= filling a hole in the Dirac sea).

Result (Feynman, Stückelberg): According to Dirac, we wish to describe the positron as a missing negative energy electron. This positron is a physical particle, and must move forward in time (first "born" at time t_0, and later "die" at time t_1).
But then the negative energy electrons must move backward in time! (They first "die" at time t_0, and later are "born" at time t_1.) In the next Section, we will see how this can be realized with Green functions (propagators).

13 Green function (propagator) for the Dirac equation

Remember: The free Dirac equation (in coordinate space) was [2]

$$(i\not\partial - m\,)\; \psi(x) = 0 \tag{13.1}$$

[2]From here, we will use "natural system of units", where $\hbar = c = 1$. We will also use Dirac's delta-function $\delta^{(4)}(x-x)$, which is doing the following under an integral:

$$\int \mathrm{d}^4x'\, F(x')\, \delta^{(4)}(x-x') = F(x)$$

i.e., it "filters out" the value at $x' = x$ of any function $F(x')$. The Fourier transform of the delta-function is a constant equal to 1, see Eq.(13.4) below.

The Green function for the Dirac equation [or: the Green function for the operator $(i\partial\!\!\!/ - m\,)$], called $S(x-x')$, is then defined by the wave equation

$$(i\partial\!\!\!/_x - m\,)\; S(x-x') = \delta^{(4)}(x-x') \tag{13.2}$$

To solve this equation, we make a Fourier transformation to momentum space:

$$\begin{aligned} S(x-x') &= \int \frac{\mathrm{d}^4p}{(2\pi)^4}\, S(p)\, e^{-ip\cdot(x-x')} && (13.3)\\ \delta^{(4)}(x-x') &= \int \frac{\mathrm{d}^4p}{(2\pi)^4}\, 1\, e^{-ip\cdot(x-x')} && (13.4)\end{aligned}$$

Then (13.2) becomes simply

$$(p\!\!\!/ - m)\; S(p) = 1 \Rightarrow S(p) = \frac{1}{p\!\!\!/ - m} = \frac{p\!\!\!/ + m}{p^2 - m^2} \tag{13.5}$$

where in the last step we multiplied $(p\!\!\!/ + m)$ in both the numerator and denominator.

<u>We will show later</u>: In order that $S(x-x')$ propagates positive energy solutions forward in time, and negative energy solutions backward in time, we need to add $i\epsilon$ (where $\epsilon = 0^+$) in the denominator to get the "Feynman propagator" S_F:

$$\begin{aligned} S_F(p) &= \frac{1}{p\!\!\!/ - m + i\epsilon} = \frac{p\!\!\!/ + m}{p^2 - m^2 + i\epsilon}\\ &= \frac{p\!\!\!/ + m}{p_0^2 - E_p^2 + i\epsilon} = \frac{p\!\!\!/ + m}{(p_0 - E_p + i\epsilon)\,(p_0 + E_p - i\epsilon)} && (13.6)\end{aligned}$$

Fourier transform back to coordinate space: From (13.3) and (13.6)

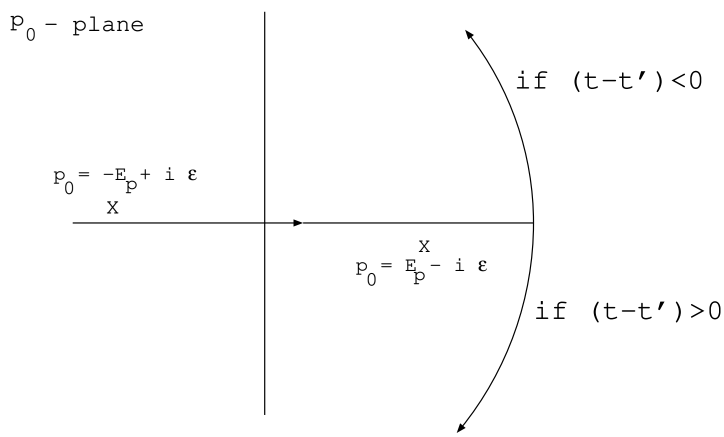
$$S_F(x-x') = \int \frac{\mathrm{d}^4p}{(2\pi)^4} \frac{p_0\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{(p_0 - E_p + i\epsilon)\,(p_0 + E_p - i\epsilon)} e^{-ip_0(t-t')}\, e^{i\vec{p}\cdot(\vec{x}-\vec{x}')} \tag{13.7}$$

In order to perform the integral over p_0, use the <u>theorem of residues</u>: We extend p_0 to the complex p_0 plane. For a closed integration contour C in the complex p_0 plane, we have the important formula

$$\oint_C \mathrm{d}p_0\, F(p_0) = 2\pi i \sum_z \text{Res}\;[F(p_0), p_0 = z] \tag{13.8}$$

Here the sum is over the poles (z) of $F(p_0)$ inside the contour C, and Res $[F(p_0), p_0 = z]$ is the <u>residue</u> of $F(p_0)$ at the pole z. For example, if $F(p_0) = \dfrac{f(p_0)}{p_0 - z}$, where $f(p_0)$ is regular (no poles), then Res $[F(p_0), p_0 = z] = f(z)$. [Note: Formula (13.8) holds for "positive" orientation of C. For negative orientation, there is a minus sign.]

Going back to our integral (13.7), we define the closed contour C in the p_0 plane by the straight line along the real axis (from $-\infty$ to $+\infty$) plus a half circle (with radius $R \to \infty$) in the upper plane or lower plane. If the integrand becomes zero on the large half circle, then the result obtained from (13.8) will be the same as the original integral $\int_{-\infty}^{\infty} \mathrm{d}p_0$.



- For $(t-t') < 0$, we close the contour in the upper plane, because in this case the factor $e^{-ip_0(t-t')}$ becomes zero for $p_0 = R(\cos\theta + i\sin\theta)$ in the limit $R \to \infty$. (Here $0 \le \theta \le \pi$). The residue at the pole $p_0 = -E_p + i\epsilon$, which is inside C, is calculated as

$$\begin{aligned}&\mathrm{Res}\left[\frac{p_0\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{(p_0 - E_p + i\epsilon)\,(p_0 + E_p - i\epsilon)}\, e^{-ip_0(t-t')}\,,\ p_0 = -E_p + i\epsilon\right]\\ &= \frac{-E_p\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{-2E_p}\, e^{iE_p(t-t')}\end{aligned}$$

- For $(t-t') > 0$, we close the contour in the lower plane, because in this case the factor $e^{-ip_0(t-t')}$ becomes zero for $p_0 = R(\cos\theta - i\sin\theta)$ in the limit $R \to \infty$. (Again $0 \le \theta \le \pi$.) The residue at the pole $p_0 = E_p - i\epsilon$, which is inside C, is calculated as

$$\begin{aligned}&\mathrm{Res}\left[\frac{p_0\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{(p_0 - E_p + i\epsilon)\,(p_0 + E_p - i\epsilon)}\, e^{-ip_0(t-t')}\,,\ p_0 = E_p - i\epsilon\right]\\ &= \frac{E_p\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{2E_p}\, e^{-iE_p(t-t')}\end{aligned}$$

We then obtain for the propagator (13.7):

$$S_F(x-x') = -i\int \frac{\mathrm{d}^3p}{(2\pi)^3}\, e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}\, \left[\theta(t-t')\,\frac{E_p\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{2E_p}\, e^{-iE_p(t-t')} + \theta(t'-t)\,\frac{-E_p\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{2E_p}\, e^{iE_p(t-t')}\right] \tag{13.9}$$

Here $\theta(x)$ is the usual "step function", i.e., $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$.

We set $\vec{p} \to -\vec{p}$ in the second term of (13.9), and use the result for the energy projection operators (see Sect. 9)

$$
\begin{aligned}
\frac{E_p\gamma^0 - \vec{p}\cdot\vec{\gamma} + m}{2m} &= \Lambda^{(+)}(\vec{p}) = \sum_s u(\vec{p},s)\,\overline{u}(\vec{p},s) \\
\frac{-E_p\gamma^0 + \vec{p}\cdot\vec{\gamma} + m}{2m} &= \Lambda^{(-)}(\vec{p}) = -\sum_s v(\vec{p},s)\,\overline{v}(\vec{p},s)
\end{aligned}
$$

Then we get

$$
\begin{aligned}
S_F(x-x') &= -i\int \frac{\mathrm{d}^3p}{(2\pi)^3}\,\frac{m}{E_p}\left[\theta(t-t')\sum_s u(\vec{p},s)\overline{u}(\vec{p},s)\,e^{-iE_p(t-t')}\,e^{i\vec{p}\cdot(\vec{x}-\vec{x}')}\right. \\
&- \left.\theta(t'-t)\sum_s v(\vec{p},s)\overline{v}(\vec{p},s)\,e^{iE_p(t-t')}\,e^{-i\vec{p}\cdot(\vec{x}-\vec{x}')}\right] \\
&= -i\theta(t-t')\int \mathrm{d}^3p\,\sum_s\,\psi^{(+)}_{\vec{p}s}(\vec{x},t)\,\overline{\psi}^{(+)}_{\vec{p}s}(\vec{x}',t') \\
&+ i\theta(t'-t)\int \mathrm{d}^3p\,\sum_s\,\psi^{(-)}_{-\vec{p}-s}(\vec{x},t)\,\overline{\psi}^{(-)}_{-\vec{p}-s}(\vec{x}',t') \qquad (13.10)
\end{aligned}
$$

where we denoted the positive and negative energy solutions of the Dirac equation by

$$
\begin{aligned}
\psi^{(+)}_{\vec{p}s}(\vec{x},t) &= \sqrt{\frac{m}{E_p}}\,\frac{1}{(2\pi)^{3/2}}\,u(\vec{p},s)\,e^{-i(E_pt-\vec{p}\cdot\vec{x})} \\
\psi^{(-)}_{-\vec{p}-s}(\vec{x},t) &= \sqrt{\frac{m}{E_p}}\,\frac{1}{(2\pi)^{3/2}}\,v(\vec{p},-s)\,e^{i(E_pt-\vec{p}\cdot\vec{x})}
\end{aligned}
$$

The normalization of these wave functions is as follows:

$$
\int \mathrm{d}^3x\;\psi^{(a)\dagger}_{\vec{p}'s'}(\vec{x},t)\,\psi^{(b)}_{\vec{p}s}(\vec{x},t) = \delta_{ab}\,\delta^{(3)}(\vec{p}'-\vec{p})\,\delta_{s's}
$$

We then see from (13.10) that the Feynman propagator acts as a "time evolution operator" in the following sense:

$$
\begin{aligned}
i\int \mathrm{d}^3x'\;S_F(x-x')\,\gamma^0\;\psi^{(+)}_{\vec{p}s}(\vec{x}',t') &= \theta(t-t')\,\psi^{(+)}_{\vec{p}s}(\vec{x},t) \qquad (13.11) \\
i\int \mathrm{d}^3x'\;S_F(x-x')\,\gamma^0\;\psi^{(-)}_{-\vec{p}-s}(\vec{x}',t') &= -\theta(t'-t)\,\psi^{(-)}_{-\vec{p}-s}(\vec{x},t) \qquad (13.12)
\end{aligned}
$$

That is, if we have a wave function at time t', and if we act with S_F on this wave function according to the l.h.s. of (13.11) and (13.12), then we get the wave function at another time t. In this sense, we can interpret relations (13.11) and (13.12) as follows: "$S_F(x-x')$ propagates the positive energy solutions forward in time, and the negative energy solutions backward in time".

Note and home work: The above interpretation is possible only with the choice of the ϵ's according to Eq.(13.6). Using any other choice (for example, $+i\epsilon$ in both factors of (13.6)) gives other time evolutions (for example, "both positive and negative energy solutions propagate forward in time"), which are regarded as unphysical in the theory of Dirac and Feynman.

Final note: The evaluation of the remaining integral $\int \mathrm{d}^3p$ in (13.9) is very tricky, and leads to Bessel functions of second kind. If you are interested, please refer to any text book on relativistic quantum mechanics.

14 Green function in an external electromagnetic field

Note: One can confirm directly that the propagator (13.10) satisfies the equation for the Green function, Eq.(13.2). This goes as follows: Apply the operator $(i\not{\partial}_x - m\,)$ to (13.10), and use

- The Dirac equation

$$(i\not{\partial} - m\,)\,\psi(\vec{x},t) = 0$$

- The identities for the derivative of step functions

$$\begin{aligned} i\gamma^0 \frac{\partial}{\partial t}\,\theta(t-t') &= i\gamma^0\,\delta(t-t') \\ i\gamma^0 \frac{\partial}{\partial t}\,\theta(t'-t) &= -i\gamma^0\,\delta(t-t') \end{aligned}$$

- The completeness relation (for fixed time t)

$$\int \mathrm{d}^3p \sum_s \left(\psi^{(+)}_{\vec{p}s}(\vec{x},t)\,\psi^{(+)\dagger}_{\vec{p}s}(\vec{x}',t) + \psi^{(-)}_{\vec{p}s}(\vec{x},t)\,\psi^{(-)\dagger}_{\vec{p}s}(\vec{x}',t)\right) = \delta^{(3)}(\vec{x}-\vec{x}') \tag{14.1}$$

Home work: Using the above three points, confirm that (13.10) satisfies (13.2).

This observation suggests that the expression (13.10), and also (13.11), (13.12), hold more generally in the presence of a time-independent external electromagnetic field field: Using the label n (instead of $\vec{p}, s$) to label the states in an external field $A^\mu = (\phi, \vec{A})$, we have

(i) The Dirac equation (see Sect. 10)

$$(i\partial\!\!\!/ - m - qA\!\!\!/\,)\,\Psi_n(\vec{x}, t) = 0 \tag{14.2}$$

(ii) The completeness relation, for fixed time t,

$$\sum_n \left(\Psi_n^{(+)}(\vec{x}, t)\,\Psi_n^{(+)\dagger}(\vec{x}', t) + \Psi_n^{(-)}(\vec{x}, t)\,\Psi_n^{(-)\dagger}(\vec{x}', t)\right) = \delta^{(3)}(\vec{x} - \vec{x}')$$

(iii) The wave equation for the propagator

$$(i\partial\!\!\!/_x - m - qA\!\!\!/\,)\; S_F(x - x') = \delta^{(4)}(x - x') \tag{14.3}$$

Then, as explained above for the free case, the Feynman propagator can be expressed by the solutions of (14.2) as follows:

$$S_F(x - x') = -i\theta(t - t') \sum_n \Psi_n^{(+)}(\vec{x}, t)\,\overline{\Psi}_n^{(+)}(\vec{x}', t') + i\theta(t' - t) \sum_n \Psi_n^{(-)}(\vec{x}, t)\,\overline{\Psi}_n^{(-)}(\vec{x}', t') \tag{14.4}$$

The time evolution for positive energy states, and its hermite conjugate (h.c.), is

$$\begin{aligned} i\int \mathrm{d}^3x'\; S_F(x - x')\,\gamma^0\; \Psi_n^{(+)}(\vec{x}', t') &= \theta(t - t')\,\Psi_n^{(+)}(\vec{x}, t) && (14.5)\\ i\int \mathrm{d}^3x\; \overline{\Psi}_n^{(+)}(x)\,\gamma^0 S_F(x - x') &= -\theta(t - t')\,\overline{\Psi}_n^{(+)}(\vec{x}', t') && (14.6) \end{aligned}$$

where we used the h.c. of S_F with respect to the Dirac matrices: $S_F^\dagger = \gamma^0\, S_F\, \gamma^0$.

<u>Dyson equation</u> for the Green function in an external electromagnetic field:
The free Feynman propagator $S_{F0}(x-x')$ and the Feynman propagator in an external field $S_F(x-x')$ satisfy the equations

$$\begin{aligned} (i\partial\!\!\!/_x - m)\; S_{F0}(x - x') &= \delta^{(4)}(x - x') && (14.7)\\ (i\partial\!\!\!/_x - m)\; S_F(x - x') &= \delta^{(4)}(x - x') + qA\!\!\!/(x) S_F(x - x') && (14.8) \end{aligned}$$

Then $S_F(x - x')$ satisfies the following integral equation (Dyson equation):

$$\begin{aligned} S_F(x - x') &= S_{F0}(x - x') + \int \mathrm{d}^4y\, S_{F0}(x - y)\; (qA\!\!\!/(y))\; S_F(y - x') && (14.9)\\ S_F &= S_{F0} + S_{F0}\,(qA\!\!\!/)\, S_F \qquad \text{(symbolically)} && (14.10) \end{aligned}$$

Proof of (14.9): Multiply (14.9) from left by $(i\not{\partial}_x - m)$ and use (14.7):

$$(i\not{\partial}_x - m)\, S_F(x-x') = \delta^{(4)}(x-x') + (q\not{A}(x))\, S_F(x-x')$$

This agrees with (14.8), which ends the proof.

The iteration of (14.10) gives a form of "perturbation series":

$$S_F \;=\; S_{F0} + S_{F0}\,(q\not{A})\,S_{F0} + S_{F0}\,(q\not{A})\,S_{F0}\,(q\not{A})\,S_{F0} + \ldots \tag{14.11}$$

Another equivalent form of the Dyson equation (14.9) is:

$$S_F(x-x') \;=\; S_{F0}(x-x') + \int \mathrm{d}^4y\, S_F(x-y)\;(q\not{A}(y))\;S_{F0}(y-x') \tag{14.12}$$

$$S_F \;=\; S_{F0} + S_F\,(q\not{A})\,S_{F0} \qquad\qquad \text{(symbolically)} \tag{14.13}$$

The iteration (perturbation series) of (14.13) is identical to (14.11). Therefore (14.13) and (14.10) are also identical.