

## KLEIN-GORDON EQUATION IN THE FESHBACH-VILLARS REPRESENTATION

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Reference: W. Greiner: *Relativistic Quantum Mechanics (Wave Equations)*; 3rd Edition, Springer-Verlag (2000); Section 1.8.

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When we write the Klein-Gordon equation in Schrödinger form, it takes the form of a matrix equation

$$\left( i\hbar \frac{\partial}{\partial t} - H_f \right) \Psi = 0 \quad (1)$$

where

$$\Psi \equiv \begin{bmatrix} \phi \\ \chi \end{bmatrix} \quad (2)$$

$$H_f \equiv (\tau_3 + i\tau_2) \frac{\mathbf{p}^2}{2m_0} + \tau_3 m_0 c^2 \quad (3)$$

and the  $\tau_i$  are essentially the Pauli matrices

$$\tau_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}; \quad \tau_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}; \quad \tau_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad \mathbf{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (4)$$

In the non-relativistic limit, the  $\phi$  component represents a particle with positive charge and the  $\chi$  component a particle with negative charge.

$$\Psi^{(+)} \rightarrow \frac{1}{\sqrt{L^3}} \begin{bmatrix} 1 \\ -\frac{1}{4} \frac{v^2}{c^2} \end{bmatrix} \quad (5)$$

$$\Psi^{(-)} \rightarrow \frac{1}{\sqrt{L^3}} \begin{bmatrix} -\frac{1}{4} \frac{v^2}{c^2} \\ 1 \end{bmatrix} \quad (6)$$

The division into these two components isn't exact, however, unless the particle's velocity is actually zero. By applying yet another transformation, we can obtain a form of the wave function in which the separation is exact. This is known as the Feshbach-Villars representation. We define the operator

$$U \equiv \frac{(m_0c^2 + E_p) - \tau_1 (m_0c^2 - E_p)}{\sqrt{4m_0c^2E_p}} \mathbf{1} \quad (7)$$

Note that  $U$  is a  $2 \times 2$  matrix since it is defined in terms of the matrices in 4.

We then apply the transformation on  $\Psi$  to get a new two-component vector  $\Phi$  as follows

$$\Phi = U\Psi \quad (8)$$

$$\Phi^\dagger = \Psi^\dagger U^\dagger \quad (9)$$

Greiner's eqn 1.95 is incorrect; the  $\Phi$  on the RHS of each equation should be  $\Psi$ .

The operator  $U$  is *not* unitary, however, as  $U^\dagger \neq U^{-1}$ . From its definition and the fact that  $\tau_1$  and  $\mathbf{1}$  are both Hermitian, we see that  $U$  is Hermitian, so that  $U^\dagger = U$ . Greiner shows that the inverse is given by

$$U^{-1} = \tau_3 U \tau_3 \quad (10)$$

We can work out  $U^{-1}$  explicitly by using the properties of the  $\tau_i$  matrices:

$$\tau_i \tau_j = -\tau_j \tau_i = i\tau_k \quad i, j, k = 1, 2, 3 \text{ \& cyclic perms.} \quad (11)$$

$$\tau_i^2 = \mathbf{1} \quad (12)$$

In particular

$$\tau_3 \tau_1 \tau_3 = i\tau_2 \tau_3 = -\tau_1 \quad (13)$$

Therefore

$$U^{-1} = \frac{(m_0c^2 + E_p) + \tau_1 (m_0c^2 - E_p)}{\sqrt{4m_0c^2E_p}} \mathbf{1} \quad (14)$$

and the fact that  $UU^{-1} = \mathbf{1}$  can be verified by direct multiplication, shown in Greiner's eqn 1.98.

We can now examine the behaviour of  $\Phi$  for a free particle. In the earlier Schrödinger form, the free particle with positive charge is represented by

$$\Psi^{(+)} = \frac{1}{\sqrt{4m_0c^2} \sqrt{L^3 E_p}} \begin{bmatrix} m_0c^2 + E_p \\ m_0c^2 - E_p \end{bmatrix} \exp \left[ \frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{x} - E_p t) \right] \quad (15)$$

Working out  $\Phi^{(+)} = U\Psi^{(+)}$  by direct multiplication (Greiner's eqn 1.99) yields

$$\Phi^{(+)} = \frac{1}{\sqrt{L^3}} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \exp \left[ \frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{x} - E_p t) \right] \quad (16)$$

Thus  $\Phi^{(+)}$ , which represents a positively charged particle, is given by a vector entirely localized to the top component. This is true for all particle speeds, not just in the nonrelativistic limit, so it is true for a relativistic particle as well.

By doing a similar calculation (Greiner eqn 1.100) we get the result for the negative particle

$$\Phi^{(-)} = U\Psi^{(-)} = \frac{1}{\sqrt{L^3}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \exp \left[ \frac{i}{\hbar} (\mathbf{p} \cdot \mathbf{x} + E_p t) \right] \quad (17)$$

so  $\Phi^{(-)}$  is localized to the lower component.

As Greiner shows in eqns 1.101 to 1.102, the normalization condition on the original  $\Psi$  vectors remains unchanged when applied to the  $\Phi$  representation:

$$\int \Psi^\dagger \tau_3 \Psi d^3x = \int \Phi^\dagger \tau_3 \Phi d^3x = \pm 1 \quad (18)$$

We can define a generalized scalar product, or 'Φ product' as

$$\langle \Psi | \Psi' \rangle_\Phi \equiv \int \Psi^\dagger \tau_3 \Psi' d^3x \quad (19)$$

Greiner's eqn 1.103 has a typo in that the second  $\Psi$  on the RHS should be  $\Psi'$ .

This scalar product is the same as that for an ordinary two-component vector except for the insertion of the  $\tau_3$  matrix within the integral. As with 18, the  $\Phi$  product is invariant under the transformation 8, as can be shown by following the steps in Greiner's eqn 1.101 for two different vectors. The result is

$$\langle \Psi | \Psi' \rangle_\Phi = \langle \Phi | \Phi' \rangle_\Phi \quad (20)$$

Suppose there is an operator  $A$  which satisfies the condition

$$\langle \Psi | \Psi' \rangle_\Phi = \langle A\Phi | A\Phi' \rangle_\Phi \quad (21)$$

In this case, we have

$$\langle \Psi | \Psi' \rangle_{\Phi} = \int \Psi^{\dagger} \tau_3 \Psi' d^3x \quad (22)$$

$$\langle A\Phi | A\Phi' \rangle_{\Phi} = \int (A\Phi)^{\dagger} \tau_3 A\Phi' d^3x \quad (23)$$

$$= \int \Phi^{\dagger} A^{\dagger} \tau_3 A\Phi' d^3x \quad (24)$$

If we require 21 then from 20 we have

$$\int \Phi^{\dagger} A^{\dagger} \tau_3 A\Phi' d^3x = \langle \Psi | \Psi' \rangle_{\Phi} \quad (25)$$

$$= \langle \Phi | \Phi' \rangle_{\Phi} \quad (26)$$

$$= \int \Phi^{\dagger} \tau_3 \Phi' d^3x \quad (27)$$

Therefore

$$A^{\dagger} \tau_3 A = \tau_3 \quad (28)$$

Multiply by  $A^{-1}$  on the right and then by  $\tau_3$  on the left to get

$$\tau_3 A^{\dagger} \tau_3 = A^{-1} \quad (29)$$

Thus  $A$  is not unitary in the ordinary sense (which would require  $A^{\dagger} = A^{-1}$ ), but if  $A$  satisfies the condition 29 it is called ' $\Phi$  unitary'. Note that if  $[\tau_3, A] = 0$ , then  $A^{\dagger} = A^{-1}$  and  $A$  is a regular unitary operator.

Because of the normalization condition 18, the charge  $Q$  of a state  $\Psi$  is

$$Q = e \int \Psi^{\dagger} \tau_3 \Psi d^3x = e \int \Phi^{\dagger} \tau_3 \Phi d^3x \quad (30)$$

This is generalized so that we can define the mean or expectation value of an operator  $L$  by

$$\langle L \rangle = \int \Psi^{\dagger} \tau_3 L \Psi d^3x \quad (31)$$

If  $L$  represents an observable, then  $\langle L \rangle$  must be a real number, so we must have

$$\left( \int \Psi^{\dagger} \tau_3 L \Psi d^3x \right)^{\dagger} = \int \Psi^{\dagger} L^{\dagger} \tau_3^{\dagger} \Psi d^3x \quad (32)$$

$$= \int \Psi^{\dagger} \tau_3 L \Psi d^3x \quad (33)$$

Since  $\tau_3^\dagger = \tau_3$  from 4, this gives the condition

$$L^\dagger \tau_3 = \tau_3 L \quad (34)$$

and since  $\tau_3^2 = \mathbf{1}$  we can multiply on the left by  $\tau_3$  to get

$$\tau_3 L^\dagger \tau_3 = L \quad (35)$$

With the definition

$$L^H \equiv \tau_3 L^\dagger \tau_3 \quad (36)$$

the condition

$$L^H = L \quad (37)$$

is called the 'generalized hermiticity condition'. If  $[L, \tau_3] = 0$ , then  $L^\dagger = L$  and  $L$  is an ordinary Hermitian operator.

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