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

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

where

$$\mathbf{\Psi}\equiv\left[\begin{array}{c}\phi\\ \chi\end{array}\right] \tag{2}$$

$$H_f\equiv\left(\tau_3+i\tau_2\right)\frac{\mathbf{p}^2}{2m_0}+\tau_3m_0c^2 \tag{3}$$

and the τ_i are essentially the Pauli matrices

$$\tau_1=\left[\begin{array}{cc}0 & 1\\ 1 & 0\end{array}\right];\quad\tau_2=\left[\begin{array}{cc}0 & -i\\ i & 0\end{array}\right];\quad\tau_3=\left[\begin{array}{cc}1 & 0\\ 0 & -1\end{array}\right]\quad\mathbf{1}=\left[\begin{array}{cc}1 & 0\\ 0 & 1\end{array}\right] \tag{4}$$

In the non-relativistic limit, the ϕ component represents a particle with positive charge and the χ component a particle with negative charge.

$$\mathbf{\Psi}^{(+)}\rightarrow\frac{1}{\sqrt{L^3}}\left[\begin{array}{c}1\\ -\frac{1}{4}\frac{v^2}{c^2}\end{array}\right] \tag{5}$$

$$\mathbf{\Psi}^{(-)}\rightarrow\frac{1}{\sqrt{L^3}}\left[\begin{array}{c}-\frac{1}{4}\frac{v^2}{c^2}\\ 1\end{array}\right] \tag{6}$$

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

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

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

We then apply the transformation on Ψ to get a new two-component vector Φ as follows

Greiner's eqn 1.95 is incorrect; the Φ on the RHS of each equation should be Ψ.

$$\Phi = U\Psi \tag{8}$$

$$\Phi^\dagger = \Psi^\dagger U^\dagger \tag{9}$$

The operator U is *not* unitary, however, as $U^\dagger \neq U^{-1}$. From its definition and the fact that τ_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

$$U^{-1} = \tau_3 U \tau_3 \tag{10}$$

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

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

$$\tau_i^2 = \mathbf{1} \tag{12}$$

In particular

$$\tau_3\tau_1\tau_3 = i\tau_2\tau_3 = -\tau_1 \tag{13}$$

Therefore

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

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 Φ for a free particle. In the earlier Schrödinger form, the free particle with positive charge is represented by

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

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

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

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

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

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

As Greiner shows in eqns 1.101 to 1.102, the normalization condition on the original Ψ vectors remains unchanged when applied to the Φ representation:

$$\int \Psi^\dagger \tau_3 \Psi d^3x = \int \Phi^\dagger \tau_3 \Phi d^3x = \pm 1 \tag{18}$$

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

$$\left\langle \Psi \middle| \Psi' \right\rangle_\Phi \equiv \int \Psi^\dagger \tau_3 \Psi' d^3x \tag{19}$$

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

This scalar product is the same as that for an ordinary two-component vector except for the insertion of the τ_3 matrix within the integral. As with 18, the Φ 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

$$\left\langle \Psi \middle| \Psi' \right\rangle_\Phi = \left\langle \Phi \middle| \Phi' \right\rangle_\Phi \tag{20}$$

Suppose there is an operator A which satisfies the condition

$$\left\langle \Psi \middle| \Psi' \right\rangle_\Phi = \left\langle A\Phi \middle| A\Phi' \right\rangle_\Phi \tag{21}$$

In this case, we have

$$\left\langle \Psi \middle| \Psi' \right\rangle_{\Phi} = \int \Psi^{\dagger} \tau_3 \Psi' d^3x \tag{22}$$

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

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

If we require 21 then from 20 we have

$$\int \Phi^{\dagger} A^{\dagger} \tau_3 A\Phi' d^3x = \left\langle \Psi \middle| \Psi' \right\rangle_{\Phi} \tag{25}$$

$$= \left\langle \Phi \middle| \Phi' \right\rangle_{\Phi} \tag{26}$$

$$= \int \Phi^{\dagger} \tau_3 \Phi' d^3x \tag{27}$$

Therefore

$$A^{\dagger} \tau_3 A = \tau_3 \tag{28}$$

Multiply by A^{-1} on the right and then by τ_3 on the left to get

$$\tau_3 A^{\dagger} \tau_3 = A^{-1} \tag{29}$$

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 'Φ 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 Ψ is

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

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

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

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

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

$$= \int \Psi^{\dagger} \tau_3 L \Psi d^3x \tag{33}$$

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

$$L^{\dagger}\tau_3=\tau_3 L \tag{34}$$

and since $\tau_3^2=\mathbf{1}$ we can multiply on the left by τ_3 to get

$$\tau_3 L^{\dagger}\tau_3=L \tag{35}$$

With the definition

$$L^H\equiv\tau_3 L^{\dagger}\tau_3 \tag{36}$$

the condition

$$L^H=L \tag{37}$$

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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