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A non-relativistic reduction of the Dirac equation in the free-particle basis

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Received 20 October 1980

Abstract. We use the non-relativistic limit of the integro-differential formulation of the Dirac equation in order to find an effective Schrödinger equation which, solved in the well known non-relativistic free-particle basis, gives approximately the same results (the probability amplitudes) as the Dirac equation for non-relativistic states written in terms of the free-particle spinors. Effective Hamiltonians for the electromagnetic and pseudoscalar interactions are derived. Comparison with the results of the Foldy-Wouthuysen method for the electromagnetic case is also achieved.

1. Introduction

In the middle of the 70s, the so-called 'pion-nucleon absorption operator ambiguity' in pion production physics required the study of the non-relativistic reduction of the Dirac equation for the pseudoscalar interaction (for a complete bibliography, see Woloshyn 1980). However, recent papers have shown that the dynamics involved in pion production physics makes these non-relativistic approximations not very appropriate and rather necessitates the direct solution of the Dirac equation (Hecking *et al* 1978). In the context of the π -N interaction, the problem of the non-relativistic reduction of the Dirac equation seems presently academic. Nevertheless, we want to point out a very interesting question which may be useful for future work in non-relativistic quantum mechanics.

The main purpose of this paper is to answer the following question: Can we construct an effective Schrödinger equation which solved in the well known basis containing the Pauli spinors χ_i

$$\phi_{(j,\boldsymbol{p},\boldsymbol{x},t)} = \chi_j (2\pi)^{-3/2} \exp[-i(et - \boldsymbol{p} \cdot \boldsymbol{x})]$$

gives approximately the same values of the probability amplitudes as the Dirac equation does for non-relativistic states expressed in terms of the positive-energy free-particle spinors

$$\Phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{(+)} = \frac{1}{(2\pi)^{3/2}} \left(\frac{e_{(p)} + m}{2e_{(p)}}\right)^{1/2} \begin{bmatrix} \chi_j \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} \\ e_{(p)} + m} \chi_j \end{bmatrix} \exp[-i(e_{(p)}t - \boldsymbol{p} \cdot \boldsymbol{x})].$$

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This kind of formulation is interesting since it would be possible to obtain some results of the Dirac theory (for a non-relativistic situation) from a Schrödinger-like equation and a state vector written in a basis commonly associated with a non-relativistic free particle. Moreover, it must be stressed that the usual non-relativistic reduction techniques such as the Pauli reduction (Messiah 1961, Bethe and Salpeter 1957) or the Foldy–Wouthuysen (Fw) transformations (Foldy and Wouthuysen 1950) do not lead to this formulation at all approximation orders of the effective Hamiltonian, as we shall see later.

Section 2 of this paper will be devoted to a method which permits such a formulation, the integro-differential (ID) method. In § 3, we shall use it for the study of the electromagnetic and the pseudoscalar interactions. Finally, we shall proceed in § 4 to the comparison of the ID and FW methods for the electromagnetic case. In this paper, the units will be such that $\hbar = c = 1$.

2. The integro-differential method

The ID method is similar in some respects to the non-relativistic reduction of the scattering (T) matrix. It consists in writing the Dirac equation in its integro-differential form, in terms of the upper (large) spinorial components, and then evaluating its non-relativistic limit. The effective Schrödinger equation will be defined in such a way to give approximately the same results when written in its integro-differential form.

The starting point is the Dirac equation (Bjorken and Drell 1964)

$$(\gamma^{0}m + \gamma^{0}\boldsymbol{\gamma} \cdot \boldsymbol{P} + V)\psi = \mathrm{i}\frac{\partial\psi}{\partial t}$$
(1)

where

$$\psi_{(\mathbf{x},t)} = \sum_{j=-1/2}^{+1/2} \int d^3 p \, a_{(j,\mathbf{p},t)} \Phi_{(j,\mathbf{p},\mathbf{x},t)}^{(+)} + \sum_{j=-1/2}^{+1/2} \int d^3 p \, b_{(j,\mathbf{p},t)}^* \Phi_{(j,\mathbf{p},\mathbf{x},t)}^{(-)} \tag{2}$$

 $\Phi_{(j,p,x,t)}^{(-)}$ and $\Phi_{(j,p,x,t)}^{(+)}$ being the negative- and positive-energy free-particle spinors respectively. We obtain from (2) and (1) the integro-differential form of the Dirac equation

$$i \frac{\partial}{\partial t} a_{(j',p',t)} = \sum_{j} \int d^{3}p \, (a_{(j,p,t)} \langle \Phi^{(+)'} | V | \Phi^{(+)} \rangle + b^{*}_{(j,p,t)} \langle \Phi^{(+)'} | V | \Phi^{(-)} \rangle)$$

$$i \frac{\partial}{\partial t} b^{*}_{(j',p',t)} = \sum_{j} \int d^{3}p \, (a_{(j,p,t)} \langle \Phi^{(-)'} | V | \Phi^{(+)} \rangle + b^{*}_{(j,p,t)} \langle \Phi^{(-)'} | V | \Phi^{(-)} \rangle).$$
(3)

It will be assumed here that we have a non-relativistic situation, where V and $\psi(\mathbf{x}, t)$ are such that if \mathbf{p} is non-relativistic and \mathbf{p}' is relativistic, we have

$$|a_{(j,p,t)}| \gg |a_{(j,p',t)}|$$
 $|a_{(j,p,t)}| \gg |b_{(j,p,t)}|$ $|a_{(j,p,t)}| \gg |b_{(j,p',t)}|$

Such an operator V has the spatial and temporal dependence suggested by Foldy and Wouthuysen (1950), that is having its eigenvalues very small compared with the mass and no time and space Fourier components comparable to or greater than m.

This allows us to put forward our first approximation

$$\psi_{(\mathbf{x},t)} \simeq \sum_{j} \int' d^{3}p \, a_{(j,\mathbf{p},t)} \Phi_{(j,\mathbf{p},\mathbf{x},t)}^{(+)}$$
(4)

and then

$$i\frac{\partial}{\partial t}a_{(j',p',t)} \simeq \sum_{j} \int' d^{3}p \, a_{(j,p,t)} \langle \Phi^{(+)'} | V | \Phi^{(+)} \rangle$$
(5)

where $\int d^3 p$ indicates that we are restricting the integration to values of non-relativistic p.

The second step is to write down equation (5) in terms of the upper (large) spinorial components, knowing that

$$V = \begin{bmatrix} V_{uu} & V_{ud} \\ V_{du} & V_{dd} \end{bmatrix} \qquad \Phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{(+)} = \begin{bmatrix} \phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{\boldsymbol{u}} \\ \phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{\boldsymbol{d}} \end{bmatrix} \qquad \text{and} \qquad \phi^{\boldsymbol{d}} = \frac{1}{e_{(p)} + m} \boldsymbol{\sigma} \cdot \boldsymbol{P} \phi^{\boldsymbol{u}}$$

 V_{uu} and ϕ^{u} being respectively 2×2 and 2×1 matrices. We then obtain

$$i\frac{\partial}{\partial t}a_{(j',p',t)} \simeq \sum_{j} \int d^{3}p \, a_{(j,p,t)} \langle \phi^{u'} | \left(V_{uu} + V_{ud} \frac{1}{e_{(p)} + m} \boldsymbol{\sigma} \cdot \boldsymbol{P} + \boldsymbol{\sigma} \cdot \boldsymbol{P} \frac{1}{e_{(p')} + m} V_{du} + \boldsymbol{\sigma} \cdot \boldsymbol{P} \frac{1}{e_{(p')} + m} V_{dd} \frac{1}{e_{(p)} + m} \boldsymbol{\sigma} \cdot \boldsymbol{P} \right) | \phi^{u} \rangle.$$

$$(6)$$

In evaluating the non-relativistic limit of equation (6), we need the following expressions and expansion:

$$\phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{u} = \left(\frac{e_{(p)} + m}{2e_{(p)}}\right)^{1/2} \frac{\chi_{j}}{(2\pi)^{3/2}} \exp[-i(e_{(p)}t - \boldsymbol{p} \cdot \boldsymbol{x})] = \left(\frac{e_{(p)} + m}{2e_{(p)}}\right)^{1/2} \phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}$$
(7)

$$P^{2}\phi_{(j,p,x,t)} = e_{(p)}^{2}\phi_{(j,p,x,t)}$$
(8)

$$e_{(p)} = m \left[1 + \left(\frac{p}{m}\right)^2 \right]^{1/2} = m \left[1 + \frac{1}{2} \left(\frac{p}{m}\right)^2 - \frac{1}{8} \left(\frac{p}{m}\right)^4 + \dots \right].$$
(9)

The use of equations (7)-(9) and the expansions of $[(e+m)/2e]^{1/2}$ and 1/(e+m) (based on equation (9)), in the non-relativistic limit of equation (6), leads to the following kind of result

$$\mathbf{i} \frac{\partial a_{(j',\mathbf{p}',t)}}{\partial t} \simeq \sum_{j} \int' \mathrm{d}^{3} p \, a_{(j,\mathbf{p},t)} \langle \phi' | v_{1} + v_{2} + \ldots + v_{n} | \phi \rangle \tag{10}$$

where v_n represents the smallest term kept in the reduction.

From (8) and (9) it is clear that we have

$$h_0\phi = \left(m + \frac{\boldsymbol{P}^2}{2m} - \frac{\boldsymbol{P}^4}{8m^3} + \ldots\right)\phi = e_{(p)}\phi.$$

If h_0 is truncated consistently at the same order of approximation as the one which led to (10), we have the following Schrödinger-like equation

$$h\hat{\psi} = (h_0 + v_1 + v_2 + \ldots + v_n)\hat{\psi} = \mathbf{i}\frac{\partial}{\partial t}\hat{\psi}$$
(11)

which gives (6) (at the order of approximation considered) if

$$\hat{\psi}_{(\mathbf{x},t)} = \sum_{j} \int' d^{3}p \, a_{(j,\mathbf{p},t)} \phi_{(j,\mathbf{p},\mathbf{x},t)}.$$
(12)

The integro-differential method is useful in the sense that the ϕ in (12) are, to all approximation orders, the non-relativistic free-particle state vector defined in § 1. This is not the case with the FW reduction technique, as we shall see in § 4.

3. Examples

Consider the electromagnetic interaction

$$V = e\varphi - \gamma^0 \boldsymbol{\gamma} \cdot e\boldsymbol{A}.$$

For this case, equation (6) is given by (to an error of $\sim (p/m)^4 e\varphi$, assuming $e\varphi \sim eA \sim (p^2/2m)$):

$$\begin{split} \mathbf{i} \frac{\partial}{\partial t} a_{(j',\mathbf{p}',t)} &\simeq \sum_{j} \int ' \mathbf{d}^{3} p \, a_{(j,\mathbf{p},t)} \Big\langle \phi' \Big| \Big(e\varphi - \frac{e}{2m} \{ \boldsymbol{\sigma} \cdot \boldsymbol{P}, \, \boldsymbol{\sigma} \cdot \boldsymbol{A} \} - \frac{e}{8m^{2}} \{ \boldsymbol{P}^{2}, \, \varphi \} \\ &+ (\boldsymbol{\sigma} \cdot \boldsymbol{P}) \frac{e\varphi}{4m^{2}} (\boldsymbol{\sigma} \cdot \boldsymbol{P}) + \frac{e}{16m^{3}} \{ \boldsymbol{P}^{2}, \, \{ \boldsymbol{\sigma} \cdot \boldsymbol{P}, \, \boldsymbol{\sigma} \cdot \boldsymbol{A} \} \} \\ &+ \frac{e}{8m^{3}} \{ \boldsymbol{P}^{2} \boldsymbol{\sigma} \cdot \boldsymbol{P}, \, \boldsymbol{\sigma} \cdot \boldsymbol{A} \} \Big) \Big| \phi \Big\rangle. \end{split}$$

After having calculated some of the anticommutators $\{, \}$, we finally obtain the following effective Schrödinger Hamiltonian

$$h_{\rm EM} = m + \frac{\mathbf{P}^2}{2m} - \frac{\mathbf{P}^4}{8m^3} + e\varphi - \frac{e}{2m}\mathbf{A}\cdot\mathbf{P} - \frac{e}{2m}\mathbf{P}\cdot\mathbf{A} - \frac{e}{2m}\boldsymbol{\sigma}\cdot(\nabla\times\mathbf{A}) + \frac{e}{8m^2}(\nabla^2\varphi) + \frac{e}{4m^2}\boldsymbol{\sigma}\cdot(\nabla\varphi)\times\mathbf{P} + \frac{e}{16m^3}\{\mathbf{P}^2, \{\boldsymbol{\sigma}\cdot\mathbf{P}, \boldsymbol{\sigma}\cdot\mathbf{A}\}\} + \frac{e}{8m^3}\{\mathbf{P}^2\boldsymbol{\sigma}\cdot\mathbf{P}, \boldsymbol{\sigma}\cdot\mathbf{A}\}.$$

If V is the pseudoscalar interaction

$$V = ig\gamma^0 \gamma^5 \tilde{\varphi}$$

we obtain to an error of about $(p/m)^4 g\tilde{\varphi}$

$$h_{\rm PS} = m + \frac{\boldsymbol{P}^2}{2m} - \frac{\boldsymbol{P}^4}{8m^3} - \frac{g}{2m}\boldsymbol{\sigma} \cdot (\boldsymbol{\nabla}\tilde{\boldsymbol{\varphi}}) + \frac{g}{16m^3} \{\boldsymbol{P}^2, \boldsymbol{\sigma} \cdot (\boldsymbol{\nabla}\tilde{\boldsymbol{\varphi}})\} + \frac{\mathrm{i}g}{8m^3} [\boldsymbol{P}^2\boldsymbol{\sigma} \cdot \boldsymbol{P}, \tilde{\boldsymbol{\varphi}}].$$

The usefulness of h_{PS} may be limited by the fact that the presence of γ^5 in V makes equation (4) a good approximation of an initially non-relativistic state vector for only a short time.

4. Discussion

Let's compare $h_{\rm EM}$ obtained previously (without the $(p/m)^3 eA$ terms) with the Hamiltonian of the FW method for the electromagnetic interaction (Bjorken and Drell 1964):

$$h_{\rm EM}^{\rm FW} = m + \frac{(\boldsymbol{P} - e\boldsymbol{A})^2}{2m} + e\varphi - \frac{e}{2m}\boldsymbol{\sigma} \cdot (\boldsymbol{\nabla} \times \boldsymbol{A}) + \frac{e}{8m^2}\boldsymbol{\nabla} \cdot \left(\boldsymbol{\nabla}\varphi + \frac{\partial}{\partial t}\boldsymbol{A}\right) + \frac{ie}{8m^2}\boldsymbol{\sigma} \cdot \left(\boldsymbol{\nabla} \times \frac{\partial}{\partial t}\boldsymbol{A}\right) + \frac{e}{4m^2}\boldsymbol{\sigma} \cdot \left(\boldsymbol{\nabla}\varphi + \frac{\partial}{\partial t}\boldsymbol{A}\right) \times \boldsymbol{P} - \frac{\boldsymbol{P}^4}{8m^3}.$$

We note that the terms containing e^2 and $\partial A/\partial t$ are missing in $h_{\rm EM}$. This difference should not surprise us since, by definition, $h_{\rm EM}$ and $h_{\rm EM}^{\rm FW}$ have to operate on different non-relativistic state vectors. $h_{\rm EM}$ must operate on the ϕ defined in § 1; with $h_{\rm EM}^{\rm FW}$, we must use $(U_{\rm FW}\Phi_{(i,p,x,t)}^{(+)})^{\rm u}$, that is the upper components of the following spinor

$$U_{FW}\Phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{(+)} = \begin{bmatrix} \left(1 + \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\frac{1}{e+m}\boldsymbol{\sigma}\cdot\boldsymbol{P} - \frac{\boldsymbol{\pi}^2}{8m^2} + \frac{e}{8m^2}\boldsymbol{\sigma}\cdot(\boldsymbol{\nabla}\times\boldsymbol{A}) + \dots\right)\boldsymbol{\phi}^{\mathsf{u}} \\ \left(\frac{1}{e+m}\boldsymbol{\sigma}\cdot\boldsymbol{P} - \frac{1}{2m}\boldsymbol{\sigma}\cdot\boldsymbol{\pi} + \frac{\mathrm{i}e}{4m^2}\boldsymbol{\sigma}\cdot\boldsymbol{E} + \dots\right)\boldsymbol{\phi}^{\mathsf{u}} \end{bmatrix}$$
(13)

where $\boldsymbol{\pi} = \boldsymbol{P} - e\boldsymbol{A}$, $\boldsymbol{E} = -\nabla \varphi - \partial \boldsymbol{A} / \partial t$, $\Phi_{(j,\boldsymbol{p},\boldsymbol{x},t)}^{(+)}$ is the free-particle Dirac spinor (see § 2) and U_{FW} the unitary operator corresponding to the FW transformations. Clearly, the two-state vectors $\boldsymbol{\phi}$ and $(U_{\text{FW}}\Phi^{(+)})^{\text{u}}$ are different except at the lowest order of approximation where then $h_{\text{EM}} = h_{\text{EM}}^{\text{FW}}$.

In order to obtain the right values of the probability amplitudes $a_{(j,p,t)}$ from h_{EM}^{FW} , we must use the vectors $(U_{FW}\Phi^{(+)})^u$ of equation (13) which differ from one approximation order to another. Similar conclusions can be drawn for $\phi_{(j,p,x,t)}^u$ (see equation (7)), the non-relativistic free-particle state vector associated with the Pauli reduction. Also, the state vectors $(U_{FW}\Phi^{(+)})^u$ depend explicitly on the interaction fields contained in the Dirac Hamiltonian (φ and eA here). In this respect, the effective Hamiltonian derived from the ID method is attractive since the state vectors associated with it (the ϕ) are always the same, no matter what the order of approximation and the interaction are.

Another practical advantage concerns the numerous studies of non-relativistic phenomena involving the ϕ : the inclusion of effects of relativistic origin consistent with the Dirac equation is a very trivial matter, since we need only to substitute the usual non-relativistic Hamiltonian by the operator h of equation (11) evaluated at the approximation order required.

Acknowledgments

The author wishes to thank Y Gingras, M Légaré, D Turcot and Professor Q Ho-Kim for helpful discussions and suggestions during the preparation of this paper. This work has been supported by scholarships from the Natural Sciences and Engineering Research Council of Canada and the Ministère de l'éducation du Québec.

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