РОСАТОМ

ГОСУДАРСТВЕННАЯ КОРПОРАЦИЯ ПО АТОМНОЙ ЭНЕРГИИ «РОСАТОМ»

РФЯЦ ВНИИЭФ

Self-adjoint second-order equations for fermions and Foldy-Wouthuysen representation

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CONTENTS

1. Introduction

2. Self-adjoint second-order equation with the spinor wave function

3. Foldy-Wouthuysen representation and chiral symmetry

3.1 Foldy-Wouthuysen chiral representation

4. Conclusions

1. INTRODUCTION

For fermions with mass m and charge e moving in an external electromagnetic field, the Dirac equation can be written as follows

$$\left(p_0 - eA_0(\mathbf{r},t)\right)\psi(\mathbf{r},t) = \left(\boldsymbol{\alpha}\left(\mathbf{p} - e\mathbf{A}(\mathbf{r},t)\right) + \beta m\right)\psi(\mathbf{r},t).$$

In equation and below, the system of units $\hbar = c = 1$ and the signature of the Minkowski space are used:

$$g_{\alpha\beta} = diag[1,-1,-1,-1].$$

$\psi(\mathbf{r},t)$ **is the bispinor wave function of a fermion;** $A_0(\mathbf{r},t), \mathbf{A}(\mathbf{r},t)$ **are potentials of the electromagnetic field;** α^k, β **are four-dimensional Dirac matrices,** $k = 1,2,3$**;** $p_0 = i\dfrac{\partial}{\partial t}, \mathbf{p} = -i\vec{\nabla}$**.**

Dirac also derived the second-order equation

$$\left[\left(p_0 - eA_0\right)^2 - \left(\mathbf{p} - e\mathbf{A}\right)^2 - m^2 + e\boldsymbol{\Sigma}\mathbf{H} - ie\boldsymbol{\alpha}\mathbf{E}\right]\psi = 0,$$

where $\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}$**,** σ^k **are two-dimensional Pauli matrices,** $\mathbf{H} = \mathrm{rot}\mathbf{A}$, $\mathbf{E} = -\dfrac{\partial \mathbf{A}}{\partial t} - \nabla A_0$ **are magnetic and electric fields. Below, we will examine stationary states when** $p_0\psi = E\psi$**, where** E **is fermion energy** $\left(\psi(\mathbf{r},t) = e^{-iEt}\psi(\mathbf{r})\right)$**.**

2. SELF-ADJOINT SECOND-ORDER EQUATION WITH THE SPINOR WAVE FUNCTION

Let the bispinor wave function has the form of

$$\psi(\mathbf{r},t)=\begin{pmatrix} u(\mathbf{r}) \\ v(\mathbf{r}) \end{pmatrix} e^{-iEt}.$$

Then

$$(E-eA_0-m)u=\boldsymbol{\sigma}(\mathbf{p}-e\mathbf{A})v,$$
$$(E-eA_0+m)v=\boldsymbol{\sigma}(\mathbf{p}-e\mathbf{A})u$$

and one can obtain equations either for the spinor u, or for the spinor v.

For the spinor $u(\mathbf{r})$, the equation has the form of

$$\left[(E-eA_0)^2-(\mathbf{p}-e\mathbf{A})^2-m^2+e\boldsymbol{\sigma}\mathbf{H}-\frac{1}{E-eA_0+m}ie\boldsymbol{\sigma}\mathbf{E}\boldsymbol{\sigma}(\mathbf{p}-e\mathbf{A})\right]u(\mathbf{r})=0.$$

In case of stationary states, the electromagnetic potentials $A_0(\mathbf{r}),A^k(\mathbf{r})$ are independent of time.

2.1 Let $A_0(\mathbf{r})=0,\ A^k(\mathbf{r})\neq 0$. Then equation for spinor is self- adjoint and

$$Eu(\mathbf{r})=\left(\pm\sqrt{m^2+(\mathbf{p}-e\mathbf{A})^2+e\boldsymbol{\sigma}\mathbf{H}}\right)u(\mathbf{r}).$$

2.2 Then, let us consider the case of $A^k(\mathbf{r})=0, A_0(\mathbf{r})\neq 0$. In this case, the latter addendum in equation for spinor $u(\mathbf{r})$ is a nonself-adjoint operator. Let us perform the non-unitary transformation of the similarity of this equation and spinor $u(\mathbf{r})$

$$\Phi(\mathbf{r})=gu(\mathbf{r}),$$

where

$$g=(E-eA_0+m)^{-1/2}.$$

As a result, equation for spinor $\Phi(\mathbf{r})$ is reduced to the form

$$g\left[(E-eA_0)^2-\mathbf{p}^2-m^2-\frac{1}{(E-eA_0+m)}i\boldsymbol{\sigma}\mathbf{E}\boldsymbol{\sigma}\mathbf{p}\right]g^{-1}\Phi(\mathbf{r})=0$$

and, finally, to

$$\left[\left[(E-eA_0)^2-\mathbf{p}^2-m^2-\frac{3}{4}\frac{1}{(E-eA_0+m)^2}\mathbf{E}^2+\frac{1}{2}\frac{1}{E-eA_0+m}\mathrm{div}\mathbf{E}+\frac{1}{E-eA_0+m}\boldsymbol{\sigma}(\mathbf{E}\times\mathbf{p})\right]\Phi(\mathbf{r})=0.\right.$$

For the central symmetric Coulomb potential, equation for spinor assumes separation of variables in spherical coordinates (r,θ,φ)

$$\Phi(r,\theta,\varphi)=F(r)\chi_\kappa^{m_\varphi}(\theta)e^{im_\varphi\varphi},$$

$\chi_\kappa^{m_\varphi}$ **are spherical spinors;** $m_\varphi=-j,-j+1,\dots j$ **is the azimuthal component of the angular momentum** j**;** κ **is the quantum number of the Dirac equation**

$$\kappa=\mp1,\mp2\ldots=\begin{cases}-(l+1), & j=l+1/2\\ l, & j=l-1/2\end{cases},$$

j,l **are quantum numbers of the angular momentum and orbital moment of a fermion.**

Taking into account the known relations

a) $\mathbf{p}^2=\mathbf{p}_r^2+\mathbf{p}_{\theta,\varphi}^2$**, where** $\mathbf{p}_r^2=-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$**,**

$$\mathbf{p}_{\theta,\varphi}^2\chi_\kappa^{m_\varphi}=-\frac{1}{r^2}\left(\frac{\partial^2}{\partial\theta^2}+\frac{1}{r^2}\operatorname{ctg}\theta\frac{\partial}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)\chi_\kappa^{m_\varphi}=\frac{\kappa(\kappa+1)}{r^2}\chi_\kappa^{m_\varphi}.$$

b) $e\boldsymbol{\sigma}(\mathbf{E}\times\mathbf{p})=-e\frac{dV}{dr}\frac{1}{r}\boldsymbol{\sigma}\mathbf{L}$**, where** $\mathbf{L}=\mathbf{r}\times\mathbf{p}$ **is the operator of the orbital moment.**

c) $-\boldsymbol{\sigma}\mathbf{L}\chi_{\kappa}^{m_{\varphi}}=(\kappa+1)\chi_{\kappa}^{m_{\varphi}}$**,**

we will obtain a Schrödinger-type equation with the effective potential for the radial function $F(r)$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)F(r)+\left((E-V)^2-m^2-\frac{\kappa(\kappa+1)}{r^2}-\frac{3}{4}\frac{\left(\frac{dV}{dr}\right)^2}{(E-V+m)^2}-\frac{1}{2}\frac{\frac{d^2V}{dr^2}}{(E-V+m)}+\frac{1}{(E-V+m)}\frac{1}{r}\frac{dV}{dr}\kappa\right)F(r)=0.$$

Here $V(\mathbf{r})=eA_0(\mathbf{r})$**.**

This equation is convenient to analyze motion of fermions in Coulomb fields of different intensity.

3. FOLDY-WOUTHUYSEN REPRESENTATION AND CHIRAL SYMMETRY

For case of $A^k(\mathbf{r}) \neq 0, A_0(\mathbf{r}) = 0$, the equation for spinor $u(\mathbf{r})$ can be written in the Hamiltonian form

$$Eu(\mathbf{r}) = Hu(\mathbf{r}), \text{ где}$$

$$H = \pm\sqrt{m^2 + (\mathbf{p} - e\mathbf{A})^2 + e\boldsymbol{\sigma}\mathbf{H}}.$$

This equation is easily compared with the Dirac equation in the Foldy-Wouthuysen representation (FW). In this representation, the bispinor wave function has formally the view

$$\psi_{FW} = \begin{pmatrix} u(\mathbf{r}) \\ 0 \end{pmatrix} e^{-iEt}, \quad E > 0,$$

$$\psi_{FW} = \begin{pmatrix} 0 \\ v(\mathbf{r}) \end{pmatrix} e^{-iEt}, \quad E < 0,$$

and the Hamiltonian is

$$H_{FW} = \beta\sqrt{m^2 + (\mathbf{p} - e\mathbf{A})^2 + e\boldsymbol{\sigma}\mathbf{H}}.$$

In case of $A^k(\mathbf{r})=0, A_0(\mathbf{r})\neq 0$ it is impossible to write equation for spinor $u(\mathbf{r})$ in the closed Hamiltonian form

$$\left[(E-eA_0)^2-(\mathbf{p}-e\mathbf{A})^2-m^2+e\boldsymbol{\sigma}\mathbf{H}-\frac{1}{E-eA_0+m}ie\boldsymbol{\sigma}\mathbf{E}\boldsymbol{\sigma}(\mathbf{p}-e\mathbf{A})\right]u(\mathbf{r})=0.$$

It can be done only by the method of successive approximations.

First, we substitute $E=E_0$ into the denominator of the last summand in this equation with $A^k(\mathbf{r})=0$. Then, we realize transformation with g_0 ensuring self-adjointness of equation. We obtain the value of the operator H_1 $(E_1\Phi(\mathbf{r})=H_1\Phi(\mathbf{r}))$. Thereafter, this process is repeated with the value of $E=H_1$ in the denominator of the last addendum in equation for spinor $u(\mathbf{r})$ up to the accuracy level needed for the physical problem under consideration.

For illustration, let $E_0=m$. Then

$$E\Phi(\mathbf{r})=H_1\Phi(\mathbf{r})=eA_0\pm\sqrt{m^2+\mathbf{p}^2+\frac{3}{16m^2}\mathbf{E}^2-\frac{1}{4m}\mathrm{div}\mathbf{E}-\frac{1}{2m}\boldsymbol{\sigma}(\mathbf{E}\times\mathbf{p})}.$$

If we restrict ourselves to summands $\sim 1/m^2$ in the expansion of the expression under the square root of this equation in the power expansion of m, we will obtain an expression, coinciding with the Foldy-Wouthuysen expansion, for the sign $(+)$ before the root.

3.1 Foldy-*Wouthuysen chiral representation*

In this case, we use matrices α^k, β in the Weyl representation widely used in the Standard model: $\beta = \gamma_0 = \rho_1$; $\alpha^k = \beta\gamma^k = \rho_3\sigma^k$; $\gamma^k = \beta\alpha^k = -i\rho_2\sigma^k$; $\gamma^5 = i\gamma^0\gamma^1\gamma^2\gamma^3 = \rho_3$; $\Sigma^i = E_{4\times4}\sigma^i$; $E_{4\times4}$ is the unit matrix.

If we present bispinor ψ as

$$\psi(\mathbf{r},t) = \begin{pmatrix} \psi_L(\mathbf{r}) \\ \psi_R(\mathbf{r}) \end{pmatrix} e^{-iEt},$$

then the summand βm in the Dirac equation mixes spinors $\psi_L(\mathbf{r}), \psi_R(\mathbf{r})$ and the Dirac equation with the non-zero mass of fermions does not possess chiral symmetry.

Conversely, in second-order equation there are no summands mixing spinors ψ_L, ψ_R and it can be written as

$$\left[\left(p_0 - eA_0\right)^2 - \left(\mathbf{p} - e\mathbf{A}_0\right)^2 - m^2 + \boldsymbol{\sigma}\mathbf{H} - ie\boldsymbol{\sigma}\mathbf{E}\right]\psi_L = 0,$$

$$\left[\left(p_0 - eA_0\right)^2 - \left(\mathbf{p} - e\mathbf{A}_0\right)^2 - m^2 + \boldsymbol{\sigma}\mathbf{H} + ie\boldsymbol{\sigma}\mathbf{E}\right]\psi_R = 0.$$

Earlier, similar equations were examined by Feynman and Gell-Mann. By using the above equations, all effects of quantum electrodynamics are reproduced with supplementary hypothesis that electrons and positrons are produced or annihilated in pairs.

These equations are chiral-symmetric. Presence or absence of fermion mass will have no effect on chiral symmetry of the equations.

Noteworthy that these equations allow obtaining a closed expression for the Hamiltonian FW in chiral representation.

Indeed, it follows from the equations

$$p_0 \psi_{FW}(\mathbf{r},t) = H_{FW} \psi_{FW}(\mathbf{r},t),$$

where for stationary states

$$\psi_{FW} = \begin{pmatrix} \psi_L \\ 0 \end{pmatrix} e^{-iEt}, \quad E > 0,$$

$$\psi_{FW} = \begin{pmatrix} 0 \\ \psi_R \end{pmatrix} e^{iEt}, \quad E < 0.$$

$$H_{FW} = eA_0 + \gamma_5 \sqrt{m^2 + (\mathbf{p} - e\mathbf{A})^2 + e\boldsymbol{\sigma}\mathbf{H} - ie\boldsymbol{\alpha}\mathbf{E}}.$$

For Hamiltonian, another representation of wave functions is also possible

$$\psi_{FW} = \begin{pmatrix} 0 \\ \psi_R \end{pmatrix} e^{-iEt}, \quad E > 0,$$

$$\psi_{FW} = \begin{pmatrix} \psi_L \\ 0 \end{pmatrix} e^{iEt}, \quad E < 0.$$

4. CONCLUSIONS

4.1 **Self- adjoint second-order equations with spinor wave functions were obtained for description of quantum-mechanical motion of fermions. The relationship was shown between these equations and the Schrödinger -type equations with effective potentials and the Dirac equation in the Foldy-Wouthuysen representation.**

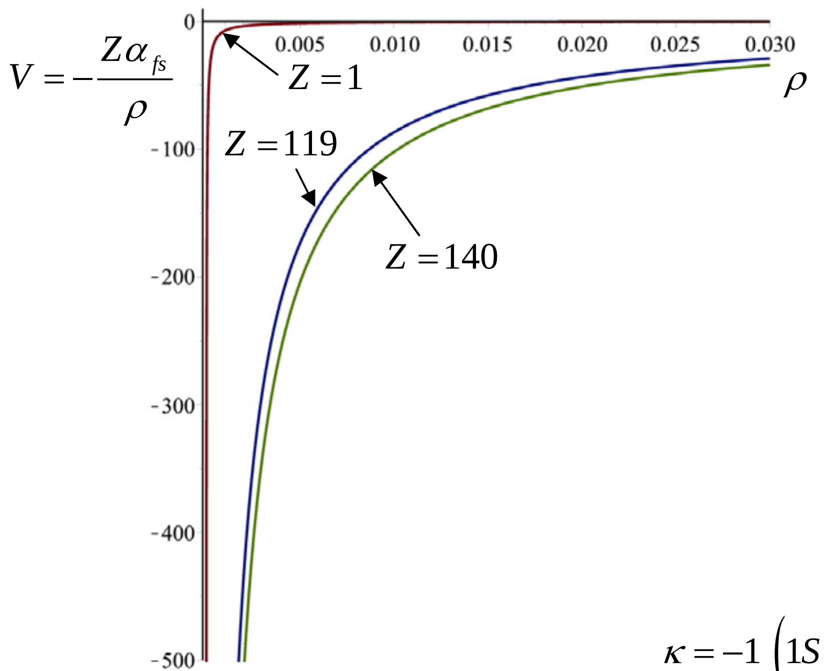
4.2 **By using four-dimensional matrices $\gamma^0, \gamma^k, \gamma^5$ in the Dirac-Pauli representation, the reason for absence of the closed FW transformation was shown at non-zero scalar potential of the electromagnetic field $A_0(\mathbf{r}, t)$. On the contrary, by using matrices $\gamma^0, \gamma^k, \gamma^5$ in chiral representation, there is a closed expression for the FW Hamiltonian in case of the general expression for the electromagnetic field $A^0(\mathbf{r}, t), A^k(\mathbf{r}, t)$. At that, the second-order equations with spinor wave functions possess chiral symmetry irrespective of presence or absence of fermion mass.**

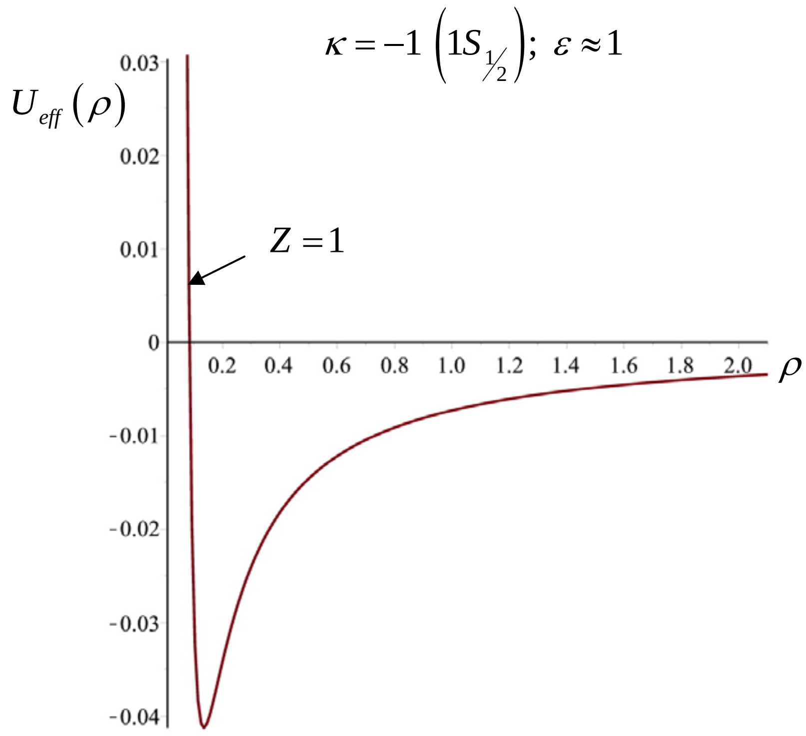
4.3 **By obtaining the self-adjoint Schrödinger-type equations with effective potentials for real radial wave functions, it is necessary to perform non-unitary similarity transformations, which can lead to new physical consequences.**

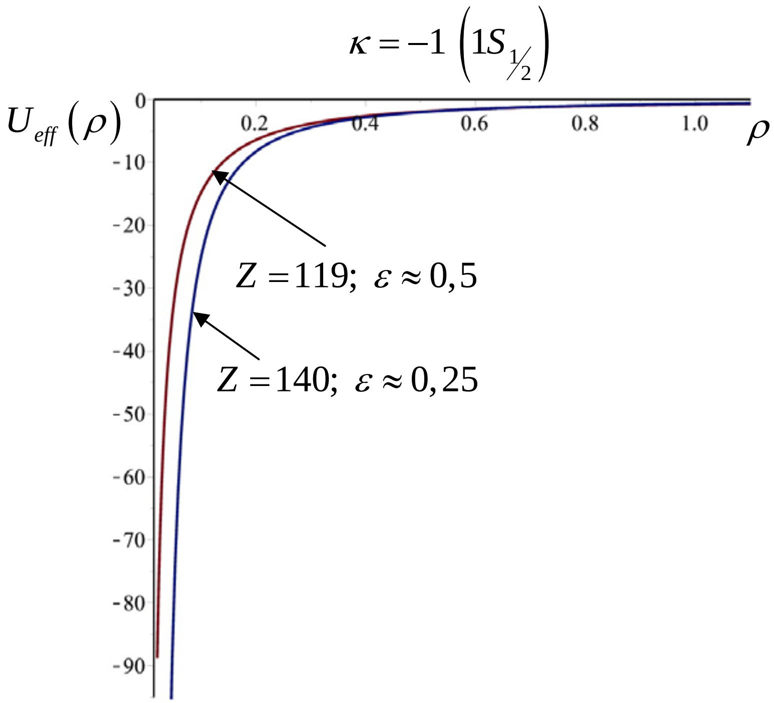
Let us note two of them:

4.3.1 **By analyzing the Schrödinger-type equation with the effective Coulomb potential, it is easy to single out three domains as** Z **variation in the source Coulomb field** $V(r) = -Ze^2/r$**:**

For the ground state $1S_{1/2}$ **in the first domain** $1 \le Z < \frac{Z \cdot 137\sqrt{3}}{2} \approx 118{,}7$ **as** $r \to 0$ **there exists the positive barrier** $\sim 1/r^2$ **with a subsequent potential well. In the second domain of** Z $(119 \le Z \le 137)$ **variation, the potential well** $\sim K/r^2$ **persists where the coefficient is** $K \le 1/8$**. This assumes the possibility of existence of fermion stationary bound states. In the third domain with** $Z > 137$**, there exists the potential well with the coefficient** $K > 1/8$**, which testifies to implementation of the mode of a particle "fall" to the center.**







$$U_{eff}\Big|_{\rho\to 0} = -\frac{\left(Z\alpha_{fs}\right)^2 - 3/4 + \left(1-\kappa^2\right)}{2\rho^2}$$

4.3.2 **Real radial wave functions of the Dirac equation in the Schwarzschild, Reissner-Nordström, Kerr and Kerr-Newman external gravitational fields are square-non-integrable in the vicinity of the event horizon. During the transition to the Schrödinger -type equation with effective potentials, the radial wave functions become square-integrable in all admissible domains, with the wave functions equal to zero on event horizons.**

So, use of self- adjoint second-order equations with spinor wave functions enhances the possibilities of quantum mechanics of fermion motion in external electromagnetic and gravitational fields.

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Thank you for your attention