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On the Dirac Scattering Problem

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Abstract

We consider a method of solving the Dirac scattering problem based on an approach previously used by the authors to solve the Schrödinger scattering problem to develop a conditional exact scattering solution and an unconditional series solution. We transform the Dirac scattering problem into a form that facilitates a solution based on the relativistic Lippmann-Schwinger equation using the relativistic Green's function that is transcendental in terms of the scattered field. Using the Dirac operator, this solution is transformed further to yield a modified relativistic Lippmann-Schwinger equation that is also transcendental in terms of the scattered field. This modified solution facilitates a condition under which the solution for the scattered field is exact. Further, by exploiting the simultaneity of the two solutions available, we show that is possible to define an exact (non-conditional) series solution to the problem.

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1 The Dirac Scattering Problem

Consider the Dirac equation for the relativistic four-component wave function $\Psi(\mathbf{r},t)$ (a function of the three-dimensional space vector $\mathbf{r}$ and time t), given by [1]

$$\hat{H}_0\Psi(\mathbf{r},t) = i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t} \tag{1}$$

where, for rest mass m, velocity of light (in a perfect vacuum) c and Dirac constant $\hbar$,

$$\begin{aligned}\hat{H}_0 &:= \frac{\hbar c}{i}\left(\alpha_1\frac{\partial}{\partial x_1}+\alpha_2\frac{\partial}{\partial x_2}+\alpha_3\frac{\partial}{\partial x_3}\right)+\beta mc^2 \\ &= c\boldsymbol{\alpha}\mathbf{p}+\beta mc^2\end{aligned} \tag{2}$$

with conventional momentum and energy operators

$$\mathbf{p}\to -i\hbar\nabla, \quad E\to i\hbar\frac{\partial}{\partial t} \quad \text{and} \quad \boldsymbol{\alpha}=(\alpha_1,\alpha_2,\alpha_3),$$

$$\alpha_1=\begin{pmatrix}\mathbf{0} & \sigma_1\\ \sigma_1 & \mathbf{0}\end{pmatrix},\quad \alpha_2=\begin{pmatrix}\mathbf{0} & \sigma_2\\ \sigma_2 & \mathbf{0}\end{pmatrix},\ \alpha_3=\begin{pmatrix}\mathbf{0} & \sigma_3\\ \sigma_3 & \mathbf{0}\end{pmatrix},$$

$$\sigma_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\ \sigma_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix};\quad \beta=\begin{pmatrix}I_2 & \mathbf{0}\\ \mathbf{0} & -I_2\end{pmatrix},$$

I_2 and $\mathbf{0}$ being 2×2 dimensional identity and zero matrices, respectively. For the stationary case, equation (1) becomes

$$\hat{H}_0\psi(\mathbf{r}) = EI_4\psi(\mathbf{r}), \tag{3}$$

where $\psi(\mathbf{r})$ is a column vector with dimension 4×1 and I_4 is a 4×4 dimensional identity matrix. The solution of the time dependent Dirac equation - equation (1) - can then be taken to be of the form (for wave vector $\mathbf{k}$ and vector dot product denoted by $\cdot$)

$$\Psi(\mathbf{r},t)=\begin{pmatrix}\chi\\ \varphi\end{pmatrix}e^{i\left(\mathbf{k}\cdot\mathbf{r}-\frac{E}{\hbar}t\right)}=\psi_i(\mathbf{r})e^{-\frac{i}{\hbar}Et},$$

where χ and φ are 'Spinors' and $\psi_i(\mathbf{r})$ is a solution of the stationary equation (3), representing a 'relativistic incident wavefield'. The solution to equation (3) is then given by [2]

$$\psi_i(\mathbf{r})=\left(\frac{E+mc^2}{2E}\right)\begin{pmatrix}\phi_s\\ \frac{c\hbar\boldsymbol{\sigma}\cdot\mathbf{k}}{E+mc^2}\phi_s\end{pmatrix}e^{i\mathbf{k}\cdot\mathbf{r}} \tag{4}$$

where

$$E^2 = c^2\hbar^2k^2 + m^2c^4,$$

$$s = \pm\frac{1}{2}, \quad \phi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ \phi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

This solution to equation (3) is called the RHS (Right Hand Side) solution and is composed of a two-spinor column vector of dimension 4×1. One can, however, also consider an equation of the form [3]

$$\overline{\psi}(\mathbf{r})\left(\hat{H}_0 - EI_4\right) = 0.$$

where $\overline{\psi}$ is a row vector with dimension 1×4, and the operator $\hat{H}_0$ operates to the left, the solution being the LHS (Left Hand Side) solution.

For a potential $V(\mathbf{r})$, equation (3) takes form

$$\hat{H}\psi(\mathbf{r}) = E\psi(\mathbf{r}) \tag{5}$$

where

$$\hat{H} = c\boldsymbol{\alpha}\mathbf{p} + \beta mc^2 + V(\mathbf{r}) = \hat{H}_0 + V(\mathbf{r}) \tag{6}$$

and $V(\mathbf{r})$ is 4×4 matrix. Thus, given equation (6), equation (5) can be written in the following form

$$(\hat{H}_0 - EI_4)\psi(\mathbf{r}) = -V(\mathbf{r})\psi(\mathbf{r}). \tag{7}$$

The Dirac scattering problem can now be defined thus: Given $V(\mathbf{r})$ solve for $\psi(\mathbf{r})$.

2 Green's Function Solution

For the stationary Dirac equation - equation (3) - the corresponding Green's function is defined by

$$(\hat{H}_0 - EI_4)G(\mathbf{r}, \mathbf{r}'; E) = -\delta(\mathbf{r} - \mathbf{r}')I_4, \tag{8}$$

Let g be the non-relativistic free-space Green's function for the Helmholtz wave operator given by

$$g(\mathbf{r}|\mathbf{r}', k) = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi \mid \mathbf{r} - \mathbf{r}' \mid}, \qquad \mathbf{r}|\mathbf{r}' \equiv \mid \mathbf{r} - \mathbf{r}' \mid$$

The relativistic Green's function can then be constructed from g as given by (and as shown in Appendix A)

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{2mc^2}(\hat{H}_0 + EI_4)g(\mathbf{r}|\mathbf{r}'; k). \tag{9}$$

This result then provides the fundamental solution to equation (7) in the form of the relativistic Lippmann-Schwinger equations for the RHS and LHS solutions which are given by [4]

$$\psi(\mathbf{r}) = \psi_i(\mathbf{r}) + \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' \tag{10}$$

and

$$\overline{\psi}(\mathbf{r}) = \overline{\psi}_i(\mathbf{r}) + \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\overline{\psi}(\mathbf{r}')d\mathbf{r}'$$

respectively. Thus, If we write the wave function in terms of the sum of relativistic incident and scattered wavefield, i.e.

$$\psi(\mathbf{r}) = \psi_i(\mathbf{r}) + \psi_s(\mathbf{r})$$

then from equation (10), we obtain the following solution

$$\psi_s(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' + \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi_s(\mathbf{r}')d\mathbf{r}'. \tag{11}$$

3 Dirac Operator based Transformation

Following the method considered in [5] for the non-relativistic case, from equation (11), it is clear that upon application of the Dirac operator $\hat{H}_0 - EI_4$

$$(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}) = -V(\mathbf{r})[\psi_i(\mathbf{r}) + \psi_s(\mathbf{r})] \tag{12}$$

which yields equation (7) given that

$$(\hat{H}_0 - EI_4)\psi_i(\mathbf{r}) = 0$$

and

$$\psi(\mathbf{r}) = \psi_i(\mathbf{r}) + \psi_s(\mathbf{r}).$$

We now note that

$$(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}) = \hat{H}_0 \left[\psi_s(\mathbf{r}) + E\int G_0(\mathbf{r}, \mathbf{r}'; E)\psi_s(\mathbf{r}')d\mathbf{r}'\right] \tag{13}$$

where $G_0(\mathbf{r}, \mathbf{r}'; E)$ is a solution to the equation

$$\hat{H}_0 G_0(\mathbf{r}, \mathbf{r}'; E) = -\delta(\mathbf{r} - \mathbf{r}')I_4$$

and is defined as

$$G_0(\mathbf{r},\mathbf{r}';E) = \hat{H}_0\left(\frac{1}{4\pi \mid \mathbf{r}-\mathbf{r}' \mid}\right).$$

Thus, from equations (12) and (13) we have

$$\hat{H}_0\left[\psi_s(\mathbf{r}) + E\int G_0(\mathbf{r},\mathbf{r}';E)\psi_s(\mathbf{r}')d\mathbf{r}'\right] = -V(\mathbf{r})[\psi_i(\mathbf{r})+\psi_s(\mathbf{r})]$$

the solution to this equation being given by

$$\psi_s(\mathbf{r}) + E\int G_0(\mathbf{r},\mathbf{r}';E)\psi_s(\mathbf{r}')d\mathbf{r}' = \int G_0(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')[\psi_i(\mathbf{r}')+\psi_s(\mathbf{r}')]d\mathbf{r}' \tag{14}$$

Rearranging equation (14) we obtain

$$\psi_s(\mathbf{r}) = \int G_0(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' + \int G_0(\mathbf{r},\mathbf{r}';E)[V(\mathbf{r}')-EI_4]\psi_s(\mathbf{r}')]d\mathbf{r}' \tag{15}$$

Both equations (11) and (15) are transcendental with regard to the relativistic scattered field $\psi_s(\mathbf{r})$ and can be solved on an iterative basis, e.g. for equation (15)

$$\psi_s(\mathbf{r}) = \int G_0(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}'$$

$$+\iint G_0(\mathbf{r},\mathbf{r}';E)[V(\mathbf{r}')-EI_4]G_0(\mathbf{r}',\mathbf{r}'';E)V(\mathbf{r}'')\psi_i(\mathbf{r}'')d\mathbf{r}''d\mathbf{r}' + ...$$

Such iterative solutions are conditional upon a convergence criteria. However, through the transformation method discussed in this section, equation (15) provides a conditional but exact scattering solution as shown in the following section.

4 Condition for an Exact Scattering Solution

Both equations (11) and (15) are exact transformations of equation (7) into integral equation form given that $\psi(\mathbf{r}) = \psi_i(\mathbf{r})+\psi_s(\mathbf{r})$ where $\psi_i(\mathbf{r})$ is a solution to the equation (10). Both equations are transcendental in $\psi_s(\mathbf{r})$ and as such do not possess an exact solution. However, unlike equation (11), equation (15) provides us with a non-conventional condition under which its transcendental characteristics are eliminated. Through inspection of equation (15), it is clear that if

$$V(\mathbf{r}) - EI_4 = 0$$

then

$$\psi_s(\mathbf{r}) = \int G_0(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' \tag{16}$$

which is an exact solution to the problem, the exact scattered field being given by equation (16). The potential energy is taken to be a constant equal to the energy of a relativistic particle which may be over a region of compact support, i.e.$\mathbf{r} \in \mathbb{R}^3$.

5 Simultaneity of Equations (11) and (15) and a Non-conditional Series Solution

Equations (11) and (15) are simultaneous integral equations for $\psi_s(\mathbf{r})$ as compounded in the following theorem.

Theorem 5.1

The simultaneity of equations (11) and (15) is consistent with equation (7) given that $\psi(\mathbf{r}) = \psi_i(\mathbf{r}) + \psi_s(\mathbf{r})$ and

$$(\hat{H}_0 - EI_4)\psi_i(\mathbf{r}) = 0$$

Proof

Subtracting equation (15) from equation (11) is clear that

$$0 = \int G_0(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' + \int G_0(\mathbf{r}, \mathbf{r}'; E)[V(\mathbf{r}') - EI_4]\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$- \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi_i(\mathbf{r}')d\mathbf{r}' - \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi_s(\mathbf{r}')d\mathbf{r}',$$

so that after collecting terms, we can write

$$0 = \int G_0(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' - \int EG_0(\mathbf{r}, \mathbf{r}'; E)\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$- \int G(\mathbf{r}, \mathbf{r}'; E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' = - \int G_0(\mathbf{r}, \mathbf{r}'; E)(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$- \int EG_0(\mathbf{r}, \mathbf{r}'; E)\psi_s(\mathbf{r}')d\mathbf{r}' + \int G(\mathbf{r}, \mathbf{r}'; E)(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}')d\mathbf{r}$$

$$= - \int G_0(\mathbf{r}, \mathbf{r}'; E)\hat{H}_0\psi_s(\mathbf{r}')d\mathbf{r}' + \int G(\mathbf{r}, \mathbf{r}'; E)(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}')d\mathbf{r}',$$

Using the definition of Green's function we can complete the proof by writing the result in the following form:

$$0 = -\int \hat{H}_0^{-1}\hat{H}_0 G_0(\mathbf{r},\mathbf{r}';E)\hat{H}_0\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$+\int (\hat{H}_0 - EI_4)^{-1}(\hat{H}_0 - EI_4)G(\mathbf{r},\mathbf{r}';E)(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$= \hat{H}_0^{-1}\int \delta(\mathbf{r}-\mathbf{r}')I_4\hat{H}_0\psi_s(\mathbf{r}')d\mathbf{r}' - (\hat{H}_0 - EI_4)^{-1}\int \delta(\mathbf{r}-\mathbf{r}')I_4(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}')d\mathbf{r}'$$

$$= \hat{H}_0^{-1}\hat{H}_0\psi_s(\mathbf{r}) - (\hat{H}_0 - EI_4)^{-1}(\hat{H}_0 - EI_4)\psi_s(\mathbf{r}) = 0.$$

Given that equations (11) and (15) are consistent with equation (7) we can exploit their simultaneity do develop a series solution. This is achieved by substituting equation (11) into the RHS of equation (15) and equation (15) into the RHS of equation (11) and then repeating this process *ad infinitum* as used for solving the non-relativistic scattering problem given in [5]. This result extends the available solutions to the Dirac scattering problem for non-spherically symmetric targets [6], for example, and yields a general approach for developing solutions associated with electron scattering problems in solid matter [6].

6 Conclusion

Theorem 6.1

Given that equation (11) is a solution to equation (7) without loss of generality, equation (7) can be written in the form

$$\hat{H}_0\left[\psi_s(\mathbf{r}) + E\int G_0(\mathbf{r},\mathbf{r}';E)\psi_s(\mathbf{r}')d\mathbf{r}'\right] = -V(\mathbf{r})[\psi_i(\mathbf{r}) + \psi_s(\mathbf{r})]$$

without loss of generality.

Proof

From equation (11), we can write

$$\psi_s(\mathbf{r}) = \int G(\mathbf{r},\mathbf{r}';E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'$$

where

$$\psi_s(\mathbf{r}) = \psi(\mathbf{r}) - \psi_i(\mathbf{r})$$

Let $Q(\mathbf{r},\mathbf{s};E)$ be an auxiliary matrices function such that

$$\int Q(\mathbf{r},\mathbf{s};E)\psi_s(\mathbf{s})d\mathbf{s} = \int Q(\mathbf{r},\mathbf{s};E)\int G(\mathbf{s},\mathbf{r}';E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'d\mathbf{s}$$

Taking the Dirac operator of this equation,

$$\hat{H}_0\left[\int Q(\mathbf{r},\mathbf{s};E)\psi_s(\mathbf{s})d\mathbf{s}\right] = \hat{H}_0\left[\int Q(\mathbf{r},\mathbf{s};E)\int G(\mathbf{s},\mathbf{r}';E)V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}'d\mathbf{s}\right]$$

$$= \int \hat{H}_0\left[\int Q(\mathbf{r},\mathbf{s};E)G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}\right]V(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' = -V(\mathbf{r})\psi(\mathbf{r}) \tag{17}$$

provided

$$\hat{H}_0\left[\int Q(\mathbf{r},\mathbf{s};E)G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}\right] = -\delta(\mathbf{r}'-\mathbf{r})I_4 \tag{18}$$

Lemma 6.1

The solution to equation (18) is

$$Q(\mathbf{r},\mathbf{s};E) = \delta(\mathbf{s}-\mathbf{r})I_4 + EG_0(\mathbf{r},\mathbf{s};E) \tag{19}$$

Proof

Substituting equation (19) into equation (18),

$$\hat{H}_0\left\{\int \left[\delta(\mathbf{s}-\mathbf{r})I_4 + EG_0(\mathbf{r},\mathbf{s};E)\right]G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}\right\}$$

$$= \hat{H}_0\left[\int \delta(\mathbf{s}-\mathbf{r})G(\mathbf{s},\mathbf{r}';E)d\mathbf{s} + E\int G_0(\mathbf{r},\mathbf{s};E)G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}\right]$$

$$= \hat{H}_0\left(G(\mathbf{r},\mathbf{r}';E) + E\int G_0(\mathbf{r},\mathbf{s};E)G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}\right)$$

$$= \hat{H}_0 G(\mathbf{r},\mathbf{r}';E) + E\int \hat{H}_0 G_0(\mathbf{r},\mathbf{s};E)G(\mathbf{s},\mathbf{r}';E)d\mathbf{s}$$

$$= \left(\hat{H}_0 - EI_4\right)G(\mathbf{r},\mathbf{r}';E) + EG(\mathbf{r},\mathbf{r}';E) - EG(\mathbf{r},\mathbf{r}';E) = -\delta(\mathbf{r}-\mathbf{r}')I_4.$$

Finally, given equations (19) and (17),

$$\hat{H}_0\left[\int Q(\mathbf{r},\mathbf{s};E)\psi_s(\mathbf{s})d\mathbf{s}\right] = \hat{H}_0\left\{\int \left[\delta(\mathbf{s}-\mathbf{r})I_4 + EG_0(\mathbf{r},\mathbf{s};E)\right]\psi_s(\mathbf{s})d\mathbf{s}\right\}$$

$$= \hat{H}_0\left[\psi_s(\mathbf{r},E) + E\int G_0(\mathbf{r},\mathbf{r}';E)\psi_s(\mathbf{s})d\mathbf{r}'\right]$$

so that

$$\hat{H}_0\left[\psi_s(\mathbf{r},E) + E\int G_0(\mathbf{r},\mathbf{r}';E)\psi_s(\mathbf{s})d\mathbf{r}'\right] = -V(\mathbf{r})\psi(\mathbf{r}).$$

7 Appendix A: Derivation of the Relativistic Green's Function

Let g be the non-relativistic free-space Green's function (for the Helmholtz wave operator) given by

$$g(\mathbf{r}|\mathbf{r}', k) = \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi \mid \mathbf{r}-\mathbf{r}' \mid}, \qquad \mathbf{r}|\mathbf{r}' \equiv \mid \mathbf{r}-\mathbf{r}' \mid .$$

The relativistic Green's function can be constructed from this function to yield

$$G(\mathbf{r}, \mathbf{r}'; E) = \frac{1}{2mc^2}(\hat{H}_0 + EI_4) g(\mathbf{r}|\mathbf{r}'; k).$$

To derive this result we first consider the identity

$$(\hat{H}_0 - EI_4)(\hat{H}_0 + EI_4) = \hat{H}_0^2 - E^2 I_4$$
$$= c^2(\boldsymbol{\alpha}\mathbf{p})^2 + mc^3(\boldsymbol{\alpha}\mathbf{p}\beta + \beta\boldsymbol{\alpha}\mathbf{p}) + m^2c^4\beta^2 - E^2 I_4.$$

We can now simplify this result on a term by term basis as follows:

(i) $c^2(\boldsymbol{\alpha}\mathbf{p})^2 = c^2\mathbf{p}^2 = c^2(-i\hbar\nabla)^2 = -c^2\hbar^2\nabla^2$

(ii) It is easy to verify that for any 4×4 matrix

$$\beta M + M\beta = 2\begin{pmatrix} m_{11} & 0 \\ 0 & -m_{22} \end{pmatrix},$$

where

$$M = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

m_{ij} being 2×2 matrices. With $M = \boldsymbol{\alpha}\mathbf{p}$ it follows that

$$(\boldsymbol{\alpha}\mathbf{p})\beta + \beta(\boldsymbol{\alpha}\mathbf{p}) = 0$$

(iii) $\beta^2 = I_4$.

Using identities (i)-(iii),

$$(\hat{H}_0 - EI_4)(\hat{H}_0 + EI_4) = -c^2\hbar^2\nabla^2 I_4 + \left(m^2c^4 - E^2\right) I_4 = -c^2\hbar^2\left(\nabla^2 + k^2\right) I_4 \qquad (A1)$$

where

$$k^2 = \frac{E^2 - m^2c^4}{c^2\hbar^2}.$$

and using the definition of the non-relativistic Green function

$$\frac{\hbar^2}{2m}\left(\nabla^2 + k^2\right) I_4 g(\mathbf{r}|\mathbf{r}'; k) = \delta(\mathbf{r} - \mathbf{r}')I_4$$

Replacing the term $\nabla^2 + k^2$ in this equation with the result given by equation (A1) yields

$$\frac{1}{2mc^2}\left(\hat{H}_0 - EI_4\right)\left(\hat{H}_0 + EI_4\right) g(\mathbf{r}|\mathbf{r}'; k) = -\delta(\mathbf{r} - \mathbf{r}')I_4.$$

Comparing this result with the definition of the relativistic Green‘s function $G(\mathbf{r}, \mathbf{r}'; E)$ the result is obtained.

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