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Kapur–Peierls and Wigner R-matrix theories for the Dirac equation

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Abstract. An R-matrix theory for the Dirac equation is shown to exist in spite of incompleteness of a relativistic R-matrix basis on the reaction surface, a phenomenon which does not occur in the non-relativistic case. The theory is constructed for the most general boundary conditions imposed on expansion basis functions. It is shown that the incompleteness of the expansion basis on the reaction surface results in a matrix correction appearing in the eigenfunction expansion of the R-matrix. The correction vanishes in the non-relativistic limit. The approach is applied to the relativistic generalizations of the Kapur–Peierls and Wigner resonance reaction theories.

1. Introduction

The Kapur–Peierls [1] and Wigner [2] R-matrix resonance reaction theories are among the foundations of the quantum scattering theory. Therefore, it might be expected that all mathematical questions of practical importance concerning both theories have been already answered, leaving only some open problems of interest for pure mathematicians. However, this is not the case: there is an important point in both theories which has not been properly resolved by their originators. While this omission has fortunately caused no problems for non-relativistic versions of the theories, it has been a source of errors in subsequent generalizations of the Wigner theory to systems described by the Dirac equation [3, 4].

Both theories belong to the family of finite-volume eigenfunction-expansion procedures generally referred to as R-matrix methods. In these approaches the configuration space of a considered system is divided into internal and external regions, separated by a reaction surface. Generally, in the internal region all particles are close together and interact strongly. The external region is the remainder of the configuration space. In the internal region one generates a denumerable set of basis functions by solving an eigenvalue problem consisting of a wave equation with a Hamiltonian describing the system under consideration, but with physical scattering boundary conditions replaced by artificial conditions imposed on solutions at the reaction surface. Once the set of eigenfunctions to this boundary-value problem has been found, a wavefunction describing the system is expanded in this set in the internal region. Particular R-matrix procedures differ among themselves with specific choices of the boundary conditions.

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An inherent problem of any eigenfunction-expansion method is a question about completeness of the expansion basis. If the basis is generated by a Hermitian eigenvalue problem, as in the Wigner theory, its completeness *in the internal region* is guaranteed [5]. The eigenvalue problem used in the Kapur–Peierls theory was non-Hermitian but Peierls [6] showed later that also in that case the basis was complete *in the internal region*. But an immediate question arises: is the expansion basis complete *on the reaction surface*? The same question may be formulated in an alternative way: does an eigenfunction expansion of the scattering wavefunction converge to that function *on the reaction surface*? Answers to these by no means trivial questions are of fundamental importance for the theories which in their widely known forms rely on the assumption that they are positive†.

Kapur and Peierls [1] did understand the problem and to cope with it introduced *ad hoc* in a rather non-rigorous way an auxiliary function χ which Brown [8] ingeniously called later the 'Peierls demon'. The function χ, which we shall call hereafter the Kapur–Peierls function, was assumed to vanish identically in the interior of the reaction volume, to vanish on the reaction surface but to have there a non-vanishing derivative. (For a present-day physicist, the properties of the Kapur–Peierls function remind one of generalized functions.) In turn, in their paper originating the R-matrix theory Wigner and Eisenbud [2] mentioned that under some simplifying restrictions they were able to prove convergence of the eigenfunction expansion on the surface but did not present a proof. Later the subject did not attract further attention [7, 9–12] although a related problem of non-uniform convergence of a derivative series was occasionally discussed [7, 9, 13–16].

Complications arose when Rosenthal [17] pointed out that the relativistic generalization of the Wigner theory given by Goertzel [3] had been incorrect. Rosenthal indicated that in the relativistic case, a fixed-boundary-condition R-matrix basis set generated in the reaction volume by a Hermitian boundary value problem was *not* complete on the reaction surface. This observation led him to the conclusion that an R-matrix formulation of the Dirac equation was not possible [17, 18]. Shortly afterwards Halderson [19], not referring explicitly to Rosenthal's paper, questioned the validity of this conclusion and attempted to prove that the theory could be constructed. However, the proof he presented was non-rigorous and correct only for a very specific choice of a boundary condition used to generate an R-matrix basis.

Recently, we have reinvestigated the relativistic generalization of the Wigner R-matrix theory for electron–atom scattering and rediscovered Rosenthal's finding about incompleteness of the relativistic R-matrix basis on the reaction surface. However, we have been able to show that in spite of this incompleteness the relativistic R-matrix theory does exist. Preliminary results of our studies have been presented in a recent paper [20] in the context of electron–atom scattering theory‡. Here we generalize our previous results by admitting more general boundary conditions on the reaction surface. We consider particular applications of our approach to the relativistic generalizations of the Kapur–Peierls and Wigner theories.

† See, however, two papers Wigner E P 1946 *Phys. Rev.* **70** 15 and *Phys. Rev.* **70** 606 and also section V.3a of [7] where the possibility that the eigenfunction expansion did not converge to the wavefunction on the boundary was admitted.

‡ A comprehensive bibliography of applications of the relativistic R-matrix theory to atomic physics is contained in [20]. There we also showed that results of numerical calculations performed thus far in atomic physics in the framework of the relativistic R-matrix theory fortuitously were not afflicted by the error in Chang's presentation of the theory [4].

2. Preliminaries

2.1. General considerations

We consider a scattering process governed by the Dirac equation

$$\left[\hat{H} - E\right]\Psi(E, \boldsymbol{r}) = 0. \tag{1}$$

The local Hamiltonian $\hat{H}$ has the form

$$\hat{H} = -\mathrm{i}c\bar{h}\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta mc^2 + V(\boldsymbol{r}) \tag{2}$$

with the matrices $\boldsymbol{\alpha}$ and β defined as usual [21], while E is a prescribed real energy of a projectile including its rest energy mc^2. We assume that the three-dimensional physical space is divided into two parts separated by a spherical shell $\mathcal{S}$ (called hereafter a *reaction surface*) of radius ρ centred at the origin of the coordinate system. In the *inner* region $\mathcal{V}$ (or *reaction volume*), $r \leqslant \rho$, the real local spin-independent potential V may be non-central and arbitrarily complicated while in the *outer* region, $r > \rho$, the potential V is assumed to vanish (a generalization of the theory to potentials with Coulomb tails is not difficult). Our goal is to construct R-matrix theories for equation (1).

Before proceeding further, we establish a notational convention. In the following, $\boldsymbol{r}$ is the position vector of a point in the three-dimensional physical space and $\boldsymbol{n} = \boldsymbol{r}/r$ is a unit vector directed along $\boldsymbol{r}$. If the point $\boldsymbol{r}$ lies on the surface $\mathcal{S}$, i.e. $r = \rho$, we shall denote this using the symbol $\boldsymbol{\rho}$ instead of $\boldsymbol{r}$. Integration over the reaction volume will be denoted by $\langle|\rangle$ and integration over the reaction surface by $(|)$. Thus for two arbitrary four-component functions f and g we have

$$\langle f|g\rangle \equiv \int_{\mathcal{V}} \mathrm{d}^3\boldsymbol{r}\, f^+(\boldsymbol{r})g(\boldsymbol{r}) \qquad (f|g) \equiv \int_{\mathcal{S}} \mathrm{d}^2\boldsymbol{\rho}\, f^+(\boldsymbol{\rho})g(\boldsymbol{\rho}) \tag{3}$$

where the superscript $+$ means the Hermitian conjugation. Whenever integration over angular variables occurs, we shall denote this explicitly by writing $\int_{4\pi} \mathrm{d}^2\boldsymbol{n}\ldots$.

Any particular solution to equation (1) may be expanded in a basis formed by two-component spherical spinors $\Omega_{\pm\kappa\mu}$

$$\Psi(E, \boldsymbol{r}) = \sum_{\kappa\mu} \frac{1}{r}\begin{pmatrix} P_{\kappa\mu}(E, r)\mathrm{i}^l\Omega_{\kappa\mu}(\boldsymbol{n}) \\ Q_{\kappa\mu}(E, r)\mathrm{i}^{l+1}\Omega_{-\kappa\mu}(\boldsymbol{n}) \end{pmatrix}. \tag{4}$$

Here $\kappa = (2j+1)(l-j)$ is a combined parity and the total angular momentum quantum number and μ is a quantum number of the projection of the total angular momentum onto a quantization axis. The factors i^l and i^{l+1} have been explicitly included in the expansion because the functions $\mathrm{i}^l\Omega_{\kappa\mu}$ and $\mathrm{i}^{l+1}\Omega_{-\kappa\mu}$ have desirable time-reversal properties [9, 22, 23]

$$(-\mathrm{i}\sigma_2\hat{K})\,\mathrm{i}^l\Omega_{\kappa\mu}(\boldsymbol{n}) = (-)^{j-\mu}\,\mathrm{i}^l\Omega_{\kappa,-\mu}(\boldsymbol{n}) \tag{5}$$

$$(-\mathrm{i}\sigma_2\hat{K})\,\mathrm{i}^{l+1}\Omega_{-\kappa\mu}(\boldsymbol{n}) = (-)^{j-\mu}\,\mathrm{i}^{l+1}\Omega_{-\kappa,-\mu}(\boldsymbol{n}) \tag{6}$$

where

$$\sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$$

is the second Pauli matrix and $\hat{K}$ is the complex conjugation operator.

It will be convenient to use a composite index $\gamma = (\kappa\mu)$ denoting a scattering channel and to define the channel *row* matrices $\boldsymbol{\Theta}$ and $\widetilde{\boldsymbol{\Theta}}$ with elements

$$\Theta_\gamma(\boldsymbol{n}) = \begin{pmatrix} \mathrm{i}^l\Omega_{\kappa\mu}(\boldsymbol{n}) \\ 0 \end{pmatrix} \qquad \widetilde{\Theta}_\gamma(\boldsymbol{n}) = \begin{pmatrix} 0 \\ \mathrm{i}^{l+1}\Omega_{-\kappa\mu}(\boldsymbol{n}) \end{pmatrix}. \tag{7}$$

Utilizing these functions we may rewrite the expansion (4) in the form more suitable for future applications

$$\Psi(E,\boldsymbol{r}) = \sum_{\gamma}\left[\Theta_\gamma(\boldsymbol{n})\frac{P_\gamma(E,r)}{r} + \widetilde{\Theta}_\gamma(\boldsymbol{n})\frac{Q_\gamma(E,r)}{r}\right]$$
$$= \boldsymbol{\Theta}(\boldsymbol{n})\frac{\mathbf{P}(E,r)}{r} + \widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\frac{\mathbf{Q}(E,r)}{r} \tag{8}$$

where $\mathbf{P}(E,r)$ and $\mathbf{Q}(E,r)$ are *column* matrices with elements respectively $P_\gamma(E,r)$ and $Q_\gamma(E,r)$ and satisfy the radial equations

$$-c\bar{h}\left[\frac{\mathrm{d}\mathbf{Q}(E,r)}{\mathrm{d}r} - \frac{\mathcal{K}}{r}\mathbf{Q}(E,r)\right] + \left[(mc^2-E)\mathbf{I} + \mathbf{V}(r)\right]\mathbf{P}(E,r) = \mathbf{0} \tag{9}$$

$$c\bar{h}\left[\frac{\mathrm{d}\mathbf{P}(E,r)}{\mathrm{d}r} + \frac{\mathcal{K}}{r}\mathbf{P}(E,r)\right] + \left[(-mc^2-E)\mathbf{I} + \mathbf{V}(r)\right]\mathbf{Q}(E,r) = \mathbf{0}. \tag{10}$$

Here $\mathcal{K}$ is a diagonal matrix of $\{\kappa_\gamma\}$, $\mathbf{I}$ is a unit matrix while

$$\mathbf{V}(r) = \int_{4\pi}\mathrm{d}^2\boldsymbol{n}\boldsymbol{\Theta}^{+}(\boldsymbol{n})V(\boldsymbol{r})\boldsymbol{\Theta}(\boldsymbol{n}) = \int_{4\pi}\mathrm{d}^2\boldsymbol{n}\widetilde{\boldsymbol{\Theta}}^{+}(\boldsymbol{n})V(\boldsymbol{r})\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n}) \tag{11}$$

is a Hermitian potential matrix which couples the channels.

2.2. The R-matrix

Let $\Psi(E,\boldsymbol{r})$ and $\Psi'(E,\boldsymbol{r})$ be two particular solutions to the Dirac equation (1) corresponding to the same real energy E. Applying the Gauss integration theorem one has

$$\langle\hat{H}\Psi'|\Psi\rangle - \langle\Psi'|\hat{H}\Psi\rangle = (\Psi'|\,\mathrm{i}c\bar{h}\boldsymbol{n}\cdot\boldsymbol{\alpha}\Psi). \tag{12}$$

In virtue of the reality of E the left-hand side of this equation vanishes. Performing the surface integration on the right-hand side we get

$$0 = (\Psi'|\,\mathrm{i}c\bar{h}\boldsymbol{n}\cdot\boldsymbol{\alpha}\Psi) = c\bar{h}\left[\mathbf{P}'^{+}(E,\rho)\mathbf{Q}(E,\rho) - \mathbf{Q}'^{+}(E,\rho)\mathbf{P}(E,\rho)\right]. \tag{13}$$

This equation implies the following linear homogeneous relation between $\mathbf{P}(E,\rho)$ and $\mathbf{Q}(E,\rho)$

$$-\frac{\bar{h}^2}{2m\rho}\boldsymbol{\mathcal{R}}^{-1}(E,\rho)\mathbf{P}(E,\rho) + c\bar{h}\mathbf{Q}(E,\rho) = \mathbf{0} \tag{14}$$

where $\boldsymbol{\mathcal{R}}(E,\rho)$ is a Hermitian matrix. (Hermicity of $\boldsymbol{\mathcal{R}}(E,\rho)$ follows immediately from substitution of equation (14) into equation (13).) The constant factors in equation (14) have been chosen for future convenience. In the more general notation the boundary condition (14) is

$$\int_{4\pi}\mathrm{d}^2\boldsymbol{n}'\left[-\frac{\bar{h}^2}{2m\rho}\boldsymbol{\Theta}(\boldsymbol{n})\boldsymbol{\mathcal{R}}^{-1}(E,\rho)\boldsymbol{\Theta}^{+}(\boldsymbol{n}') + \mathrm{i}c\bar{h}\delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1+\beta}{2}\boldsymbol{n}'\cdot\boldsymbol{\alpha}\right]\Psi(E,\boldsymbol{\rho}') = 0$$
$$\text{on } \mathcal{S}. \tag{15}$$

We observe that equation (15) is not a unique way of writing the boundary condition it expresses since equation (14) may be rewritten as

$$2m\rho c^2\boldsymbol{\mathcal{R}}(E,\rho)\mathbf{Q}(E,\rho) - c\bar{h}\mathbf{P}(E,\rho) = \mathbf{0} \tag{16}$$

where again the constant factors have been chosen for future convenience. This shows that the boundary condition implied by equation (15) may also be written in the form

$$\int_{4\pi} \mathrm{d}^2\boldsymbol{n}' \left[2m\rho c^2 \widetilde{\boldsymbol{\Theta}}(\boldsymbol{n}) \boldsymbol{\mathcal{R}}(E,\rho) \widetilde{\boldsymbol{\Theta}}^{+}(\boldsymbol{n}') + \mathrm{i}c\hbar\delta(\boldsymbol{n}-\boldsymbol{n}') \frac{1-\beta}{2} \boldsymbol{n}' \cdot \boldsymbol{\alpha} \right] \Psi(E,\boldsymbol{\rho}') = 0 \qquad \text{on } \mathcal{S}. \tag{17}$$

We have already seen that the matrix $\boldsymbol{\mathcal{R}}(E,\rho)$ is Hermitian. Now we shall prove that it has an additional symmetry property. To show this we observe that the Hamiltonian $\hat{H}$ defined by equation (2) is invariant under the time-reversal transformation $\hat{T} = -\mathrm{i}\Sigma_2\hat{K}$, where Σ_2 is the second Dirac spin matrix, and that the energy E is real. This implies that if the function Ψ given by the expansion (4) is a solution to equation (1) then its time-reversed conjugate

$$\hat{T}\Psi(E,\boldsymbol{r}) = \sum_{\kappa\mu} (-)^{j-\mu} \frac{1}{r} \begin{pmatrix} P^{*}_{\kappa\mu}(E,r)\mathrm{i}^{l}\Omega_{\kappa,-\mu}(\boldsymbol{n}) \\ Q^{*}_{\kappa\mu}(E,r)\mathrm{i}^{l+1}\Omega_{-\kappa,-\mu}(\boldsymbol{n}) \end{pmatrix} \tag{18}$$

where the asterisk denotes the complex conjugation, is also a solution to equation (1) corresponding to the same energy E. This means that the radial components of the latter function must satisfy the relation (14) which gives

$$\mathcal{R}_{\kappa\mu;\kappa'\mu'}(E,\rho) = (-)^{(j-j')-(\mu-\mu')} \mathcal{R}^{*}_{\kappa,-\mu;\kappa',-\mu'}(E,\rho) \tag{19}$$

or after utilizing the Hermicity property of $\boldsymbol{\mathcal{R}}(E,\rho)$

$$\mathcal{R}_{\kappa\mu;\kappa'\mu'}(E,\rho) = (-)^{(j-j')-(\mu-\mu')} \mathcal{R}_{\kappa',-\mu';\kappa,-\mu}(E,\rho). \tag{20}$$

2.3. The scattering matrix

Although the matrix $\boldsymbol{\mathcal{R}}(E,\rho)$ contains all the information about processes taking place in the reaction volume, the central role in the theory is played by the *scattering* (or *collision*) matrix $\mathbf{S}(E)$. Consider the particular solution $\Psi_{\kappa\mu}(E,\boldsymbol{r})$ to the Dirac equation (1) that, in the *external* region, contains an incoming wave in channel $\kappa\mu$ and outgoing waves in all channels

$$\Psi_{\kappa\mu}(E,\boldsymbol{r}) = N\frac{1}{r} \begin{pmatrix} I_{\kappa}(E,r)\mathrm{i}^{l}\Omega_{\kappa\mu}(\boldsymbol{n}) \\ \widetilde{I}_{\kappa}(E,r)\mathrm{i}^{l+1}\Omega_{-\kappa\mu}(\boldsymbol{n}) \end{pmatrix} - \sum_{\kappa'\mu'} N\frac{1}{r} \begin{pmatrix} O_{\kappa'}(E,r)\mathrm{i}^{l'}\Omega_{\kappa'\mu'}(\boldsymbol{n}) \\ \widetilde{O}_{\kappa'}(E,r)\mathrm{i}^{l'+1}\Omega_{-\kappa'\mu'}(\boldsymbol{n}) \end{pmatrix} S_{\kappa'\mu',\kappa\mu}(E) \qquad \text{for } r \geqslant \rho. \tag{21}$$

The factor

$$N = \frac{1}{\sqrt{2c}} \sqrt[4]{\frac{E+mc^2}{E-mc^2}} \tag{22}$$

normalizes the incoming and outgoing partial waves to unit flux crossing any sphere centred at the origin. The radial functions I_κ, O_κ, $\widetilde{I}_\kappa$ and $\widetilde{O}_\kappa$ are related to the Riccati–Hankel functions $\hat{h}^{(\mp)}_l$ [24]

$$I_{\kappa}(E,r) = -\mathrm{i}\hat{h}^{(-)}_{l}(kr) \xrightarrow{r\to\infty} +\exp\left[-\mathrm{i}\left(kr - \frac{\pi l}{2}\right)\right] \tag{23}$$

$$O_{\kappa}(E,r) = +\mathrm{i}\hat{h}^{(+)}_{l}(kr) \xrightarrow{r\to\infty} +\exp\left[\mathrm{i}\left(kr - \frac{\pi l}{2}\right)\right] \tag{24}$$

$$\widetilde{I}_\kappa(E,r) = \pm \mathrm{i}\epsilon\sqrt{\frac{E-mc^2}{E+mc^2}}\hat{h}^{(-)}_{l\pm1}(kr) \overset{r\to\infty}{\longrightarrow} -\mathrm{i}\epsilon\sqrt{\frac{E-mc^2}{E+mc^2}}\exp\left[-\mathrm{i}\left(kr-\frac{\pi l}{2}\right)\right] \tag{25}$$

$$\widetilde{O}_\kappa(E,r) = \mp \mathrm{i}\epsilon\sqrt{\frac{E-mc^2}{E+mc^2}}\hat{h}^{(+)}_{l\pm1}(kr) \overset{r\to\infty}{\longrightarrow} +\mathrm{i}\epsilon\sqrt{\frac{E-mc^2}{E+mc^2}}\exp\left[\mathrm{i}\left(kr-\frac{\pi l}{2}\right)\right] \tag{26}$$

where $\epsilon = +1$ for $E > +mc^2$ and $\epsilon = -1$ for $E < -mc^2$ and

$$k = \frac{\sqrt{(E-mc^2)(E+mc^2)}}{c\hbar} \tag{27}$$

is a wave number of the scattered particle. In equations (25) and (26) the upper sign should be taken for $\kappa < 0$ and the lower one for $\kappa > 0$. The set of probability amplitudes $\{S_{\kappa'\mu',\kappa\mu}(E)\}$ forms the scattering matrix $\mathbf{S}(E)$.

An arbitrary solution to equation (1) at energy E may be expanded in the set $\{\Psi_\gamma\}$

$$\Psi(E,\boldsymbol{r}) = \sum_\gamma \Psi_\gamma(E,\boldsymbol{r})X_\gamma(E) \tag{28}$$

where $\{X_\gamma(E)\}$ are the expansion coefficients. Introducing a column matrix $\mathbf{X}(E)$ with elements $X_\gamma(E)$ and diagonal matrices $\boldsymbol{\mathcal{I}}(E,r)$, $\boldsymbol{\mathcal{O}}(E,r)$, $\widetilde{\boldsymbol{\mathcal{I}}}(E,r)$ and $\widetilde{\boldsymbol{\mathcal{O}}}(E,r)$ with diagonal elements defined by equations (23)–(26), in the *external* region we may rewrite the expansion (28) in the form

$$\begin{aligned}\Psi(E,\boldsymbol{r}) = {} & \boldsymbol{\Theta}(\boldsymbol{n})\frac{N\left[\boldsymbol{\mathcal{I}}(E,r)-\boldsymbol{\mathcal{O}}(E,r)\mathbf{S}(E)\right]}{r}\mathbf{X}(E) \\ & +\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\frac{N\left[\widetilde{\boldsymbol{\mathcal{I}}}(E,r)-\widetilde{\boldsymbol{\mathcal{O}}}(E,r)\mathbf{S}(E)\right]}{r}\mathbf{X}(E) \qquad \text{for } r \geqslant \rho.\end{aligned} \tag{29}$$

Consider now two solutions $\Psi(E,\boldsymbol{r})$ and $\Psi'(E,\boldsymbol{r})$ to the Dirac equation (1) corresponding to the same real energy E. We have shown in the previous subsection that on the reaction surface $\mathcal{S}$ their radial parts must satisfy the relation

$$\mathbf{P}'^{+}(E,\rho)\mathbf{Q}(E,\rho) - \mathbf{Q}'^{+}(E,\rho)\mathbf{P}(E,\rho) = 0. \tag{30}$$

In our case

$$\mathbf{P}(E,\rho) = \left[\boldsymbol{\mathcal{I}}(E,\rho)-\boldsymbol{\mathcal{O}}(E,\rho)\mathbf{S}(E)\right]\mathbf{X}(E) \tag{31}$$

and

$$\mathbf{Q}(E,\rho) = \left[\widetilde{\boldsymbol{\mathcal{I}}}(E,\rho)-\widetilde{\boldsymbol{\mathcal{O}}}(E,\rho)\mathbf{S}(E)\right]\mathbf{X}(E). \tag{32}$$

On substituting equations (31) and (32) to equation (30) and utilizing the Hermitian-conjugation relations

$$\boldsymbol{\mathcal{I}}^{+}(E,r) = \boldsymbol{\mathcal{O}}(E,r) \qquad \boldsymbol{\mathcal{O}}^{+}(E,r) = \boldsymbol{\mathcal{I}}(E,r) \tag{33}$$

$$\widetilde{\boldsymbol{\mathcal{I}}}^{+}(E,r) = \widetilde{\boldsymbol{\mathcal{O}}}(E,r) \qquad \widetilde{\boldsymbol{\mathcal{O}}}^{+}(E,r) = \widetilde{\boldsymbol{\mathcal{I}}}(E,r) \tag{34}$$

and the Wrońskian relation

$$\boldsymbol{\mathcal{O}}(E,r)\widetilde{\boldsymbol{\mathcal{I}}}(E,r) - \boldsymbol{\mathcal{I}}(E,r)\widetilde{\boldsymbol{\mathcal{O}}}(E,r) = -2\mathrm{i}\epsilon\sqrt{\frac{E-mc^2}{E+mc^2}}\mathbf{I} \tag{35}$$

we obtain

$$\mathbf{S}^{+}(E)\mathbf{S}(E) = \mathbf{I} \tag{36}$$

which means that the matrix $\mathbf{S}(E)$ is unitary. An argumentation following essentially the one presented at the end of the previous subsection shows that the matrix $\mathbf{S}(E)$ has an additional symmetry property

$$S_{\kappa\mu;\kappa'\mu'}(E) = (-)^{(j-j')-(\mu-\mu')} S_{\kappa',-\mu';\kappa,-\mu}(E). \tag{37}$$

Finally, a relation between the matrices $\mathbf{S}(E)$ and $\boldsymbol{\mathcal{R}}(E,\rho)$ may be established. Substituting equations (31) and (32) in condition (14) we obtain

$$\begin{aligned}\mathbf{S}(E) &= \boldsymbol{\mathcal{O}}^{-1}(E,\rho)[\mathbf{I} - \boldsymbol{\mathcal{R}}(E,\rho)\mathbf{L}(E,\rho)]^{-1}[\mathbf{I} - \boldsymbol{\mathcal{R}}(E,\rho)\mathbf{L}^{+}(E,\rho)]\boldsymbol{\mathcal{I}}(E,\rho) \\ &= \boldsymbol{\mathcal{I}}(E,\rho)[\mathbf{I} - \mathbf{L}^{+}(E,\rho)\boldsymbol{\mathcal{R}}(E,\rho)][\mathbf{I} - \mathbf{L}(E,\rho)\boldsymbol{\mathcal{R}}(E,\rho)]^{-1}\boldsymbol{\mathcal{O}}^{-1}(E,\rho)\end{aligned} \tag{38}$$

where

$$\mathbf{L}(E,\rho) = \left(\frac{2m\rho c}{\hbar}\right)\widetilde{\boldsymbol{\mathcal{O}}}(E,\rho)\boldsymbol{\mathcal{O}}^{-1}(E,\rho). \tag{39}$$

3. Construction and properties of an expansion basis

In the following we shall need a set of functions $\{\Phi_{\mathbf{b}K}\}$

$$\Phi_{\mathbf{b}K}(\boldsymbol{r}) = \boldsymbol{\Theta}(\boldsymbol{n})\frac{\mathbf{F}_{\mathbf{b}K}(r)}{r} + \widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\frac{\mathbf{G}_{\mathbf{b}K}(r)}{r} \tag{40}$$

that are solutions to the equation

$$\left[\hat{H} - E_{\mathbf{b}K}\right]\Phi_{\mathbf{b}K}(\boldsymbol{r}) = 0 \qquad \text{in } \mathcal{V} \tag{41}$$

augmented by a homogeneous boundary condition

$$\int_{4\pi} \mathrm{d}^2\boldsymbol{n}'\left[-\frac{\hbar^2}{2m\rho}\boldsymbol{\Theta}(\boldsymbol{n})\mathbf{b}\boldsymbol{\Theta}^{+}(\boldsymbol{n}') + \mathrm{i}c\hbar\delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1+\beta}{2}\boldsymbol{n}'\cdot\boldsymbol{\alpha}\right]\Phi_{\mathbf{b}K}(\boldsymbol{\rho}') = 0 \qquad \text{on } \mathcal{S} \tag{42}$$

or equivalently

$$\int_{4\pi} \mathrm{d}^2\boldsymbol{n}'\left[2m\rho c^2\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\mathbf{b}^{-1}\widetilde{\boldsymbol{\Theta}}^{+}(\boldsymbol{n}') + \mathrm{i}c\hbar\delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1-\beta}{2}\boldsymbol{n}'\cdot\boldsymbol{\alpha}\right]\Phi_{\mathbf{b}K}(\boldsymbol{\rho}') = 0 \qquad \text{on } \mathcal{S}. \tag{43}$$

$\mathbf{b}$ is a square, in general non-diagonal and possibly non-Hermitian, matrix. We note that in general the eigenvalues $\{E_{\mathbf{b}K}\}$ will be complex. In terms of radial column matrices, equations (42) and (43) may be respectively rewritten as

$$-\frac{\hbar^2}{2m\rho}\mathbf{b}\mathbf{F}_{\mathbf{b}K}(\rho) + c\hbar\mathbf{G}_{\mathbf{b}K}(\rho) = \mathbf{0} \tag{44}$$

and

$$2m\rho c^2\mathbf{b}^{-1}\mathbf{G}_{\mathbf{b}K}(\rho) - c\hbar\mathbf{F}_{\mathbf{b}K}(\rho) = \mathbf{0}. \tag{45}$$

In the very special case when the matrix $\mathbf{b}$ is proportional to a unit matrix, $\mathbf{b} = b\mathbf{I}$, equations (42) and (43) simplify and become

$$\frac{1+\beta}{2}\left[-\frac{\hbar^2}{2m\rho}b + \mathrm{i}c\hbar\boldsymbol{n}\cdot\boldsymbol{\alpha}\right]\Phi_{\mathbf{b}K}(\boldsymbol{\rho}) = 0 \qquad \text{on } \mathcal{S} \tag{46}$$

$$\frac{1-\beta}{2}\left[2m\rho c^2 b^{-1} + \mathrm{i}c\hbar\boldsymbol{n}\cdot\boldsymbol{\alpha}\right]\Phi_{\mathbf{b}K}(\boldsymbol{\rho}) = 0 \qquad \text{on } \mathcal{S} \tag{47}$$

since

$$\boldsymbol{\Theta}(\boldsymbol{n})\boldsymbol{\Theta}^{+}(\boldsymbol{n}') = \delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1+\beta}{2} \tag{48}$$

and

$$\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\widetilde{\boldsymbol{\Theta}}^{+}(\boldsymbol{n}') = \delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1-\beta}{2}. \tag{49}$$

The boundary condition (46) was used by Goertzel [3] and Halderson [19]. In what follows, we shall not restrict ourselves to this special case but shall consider the most general situation when $\mathbf{b}$ is non-diagonal.

A convenient way to deal with the boundary condition (42)–(45) is to write it in the form

$$\hat{\mathcal{L}}_{\mathbf{b}}\Phi_{\mathbf{b}K}(\boldsymbol{\rho}) = 0 \qquad \text{on } \mathcal{S}. \tag{50}$$

The most general form of the integral kernel $L_{\mathbf{b}}(\boldsymbol{r},\boldsymbol{r}')$ of the relativistic Bloch surface operator $\hat{\mathcal{L}}_{\mathbf{b}}$ [25, 26] corresponding to the Hamiltonian $\hat{H}$ and the boundary condition expressed by equations (42) and (43) is

$$\begin{aligned} L_{\mathbf{b}}(\boldsymbol{r},\boldsymbol{r}') = {} & \eta\,\frac{\delta(r-\rho)\delta(r'-\rho)}{\rho^2}\left[-\frac{\overline{h}^2}{2m\rho}\boldsymbol{\Theta}(\boldsymbol{n})\mathbf{b}\boldsymbol{\Theta}^{+}(\boldsymbol{n}') + \mathrm{i}c\overline{h}\delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1+\beta}{2}\boldsymbol{n}'\cdot\boldsymbol{\alpha}\right] \\ & +(1-\eta)\,\frac{\delta(r-\rho)\delta(r'-\rho)}{\rho^2} \\ & \times\left[2m\rho c^2\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\mathbf{b}^{-1}\widetilde{\boldsymbol{\Theta}}^{+}(\boldsymbol{n}') + \mathrm{i}c\overline{h}\delta(\boldsymbol{n}-\boldsymbol{n}')\frac{1-\beta}{2}\boldsymbol{n}'\cdot\boldsymbol{\alpha}\right] \end{aligned} \tag{51}$$

where η is an arbitrary real number. This specific choice of real coefficients, η and $1-\eta$, ensures that the extended (in general non-Hermitian) Hamiltonian

$$\hat{\mathcal{H}}_{\mathbf{b}} = \hat{H} + \hat{\mathcal{L}}_{\mathbf{b}} \tag{52}$$

has the property

$$\hat{\mathcal{H}}_{\mathbf{b}}^{+} = \hat{\mathcal{H}}_{\mathbf{b}^{+}}. \tag{53}$$

A proof is simple and utilizes the equalities

$$\hat{H}^{+} = \hat{H} + \mathrm{i}c\overline{h}\delta(r-\rho)\boldsymbol{n}\cdot\boldsymbol{\alpha} \tag{54}$$

and

$$L_{\mathbf{b}}^{+}(\boldsymbol{r}',\boldsymbol{r}) = L_{\mathbf{b}^{+}}(\boldsymbol{r},\boldsymbol{r}') - \mathrm{i}c\overline{h}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(r-\rho)\boldsymbol{n}\cdot\boldsymbol{\alpha} \tag{55}$$

the first of which follows from equation (12), and the latter from equation (51) and the anticommutation relation $\boldsymbol{\alpha}\beta + \beta\boldsymbol{\alpha} = 0$. With the operator $\hat{\mathcal{H}}_{\mathbf{b}}$ we may rewrite the eigenvalue problem constituted by equation (41) and the boundary condition (50) in the compact form

$$\left[\hat{\mathcal{H}}_{\mathbf{b}} - E_{\mathbf{b}K}\right]\Phi_{\mathbf{b}K}(\boldsymbol{r}) = 0 \qquad \text{in } \mathcal{V}. \tag{56}$$

Since we have admitted boundary conditions such that the extended Hamiltonian $\hat{\mathcal{H}}_{\mathbf{b}}$ may be non-Hermitian, in general the functions $\{\Phi_{\mathbf{b}K}\}$ will not be mutually orthogonal and we shall need a set of complementary biorthonormal functions $\{\Phi_{\mathbf{b}K}^{\perp}\}$ which are solutions to the equation

$$\left[\hat{\mathcal{H}}_{\mathbf{b}}^{+} - E_{\mathbf{b}K}^{*}\right]\Phi_{\mathbf{b}K}^{\perp}(\boldsymbol{r}) = 0 \qquad \text{in } \mathcal{V}. \tag{57}$$

Because of the property (53) of the extended Hamiltonian $\hat{\mathcal{H}}_{\mathbf{b}}$ the sets $\{\Phi^{\perp}_{\mathbf{b}K}\}$ and $\{\Phi_{\mathbf{b}^+K}\}$ coincide, as do the sets $\{E^*_{\mathbf{b}K}\}$ and $\{E_{\mathbf{b}^+K}\}$. Moreover, it is always possible to index the functions in such a way that

$$\Phi^{\perp}_{\mathbf{b}K}(\boldsymbol{r}) = \Phi_{\mathbf{b}^+K}(\boldsymbol{r}) \qquad E^*_{\mathbf{b}K} = E_{\mathbf{b}^+K} \tag{58}$$

and henceforth we shall take these relations for granted.

In the following we shall assume† that the functions $\{\Phi_{\mathbf{b}K}\}$ form a complete set spanning the *interior* of the reaction volume, $\mathcal{V} \setminus \mathcal{S}$. The corresponding closure relation is

$$\sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})\Phi^+_{\mathbf{b}^+K}(\boldsymbol{r}') = \delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \text{for } \boldsymbol{r}, \boldsymbol{r}' \in \mathcal{V} \setminus \mathcal{S}. \tag{59}$$

This set, however, is *not* complete on the surface $\mathcal{S}$ because of the restrictive condition (50) obeyed by the functions $\{\Phi_{\mathbf{b}K}\}$. If the point $\boldsymbol{r}'$ lies on the surface $\mathcal{S}$ (i.e. $\boldsymbol{r}' = \boldsymbol{\rho}'$), then instead of equation (59) we assume (cf equations (40) and (44))

$$\sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})\Phi^+_{\mathbf{b}^+K}(\boldsymbol{\rho}') = \frac{\delta(r-\rho)}{\rho^2}\left[\boldsymbol{\Theta}(\boldsymbol{n}) + \left(\frac{\hbar}{2m\rho c}\right)\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\mathbf{b}\right] \times \mathbf{A}_{\mathbf{b}}(\rho)\left[\boldsymbol{\Theta}^+(\boldsymbol{n}') + \left(\frac{\hbar}{2m\rho c}\right)\mathbf{b}\widetilde{\boldsymbol{\Theta}}^+(\boldsymbol{n}')\right] \qquad \text{for } \boldsymbol{r} \in \mathcal{V} \tag{60}$$

where the square matrix $\mathbf{A}_{\mathbf{b}}(\rho)$, defined formally by the relation

$$\sum_K \mathbf{F}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho) = \mathbf{A}_{\mathbf{b}}(\rho)\delta(r-\rho) \qquad r \leqslant \rho \tag{61}$$

is to be determined.

4. The eigenfunction expansion of the solution to the Dirac equation

An idea underlying the *R*-matrix theories is to expand the wave function Ψ in the *interior* of the reaction volume, $\mathcal{V} \setminus \mathcal{S}$, in the complete set of the eigenfunctions $\{\Phi_{\mathbf{b}K}\}$ of the operator $\hat{\mathcal{H}}_{\mathbf{b}}$,

$$\Psi(E, \boldsymbol{r}) = \sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})C_{\mathbf{b}K}(E) \qquad \text{in } \mathcal{V} \setminus \mathcal{S} \tag{62}$$

with the expansion coefficients $\{C_{\mathbf{b}K}(E)\}$ formally given by

$$C_{\mathbf{b}K}(E) = \langle \Phi_{\mathbf{b}^+K} | \Psi \rangle. \tag{63}$$

To find the coefficients, we add to both sides of equation (1) the term $\hat{\mathcal{L}}_{\mathbf{b}}\Psi(E, \boldsymbol{r})$, premultiply the resulting equation by $\Phi^+_{\mathbf{b}^+K}(\boldsymbol{r})$

$$\Phi^+_{\mathbf{b}^+K}(\boldsymbol{r})\left[\hat{\mathcal{H}}_{\mathbf{b}} - E\right]\Psi(E, \boldsymbol{r}) = \Phi^+_{\mathbf{b}^+K}(\boldsymbol{r})\hat{\mathcal{L}}_{\mathbf{b}}\Psi(E, \boldsymbol{r}) \tag{64}$$

postmultiply the Hermitian conjugate of equation (57) by $\Psi(E, \boldsymbol{r})$,

$$\left(\left[\hat{\mathcal{H}}^+_{\mathbf{b}} - E^*_{\mathbf{b}K}\right]\Phi_{\mathbf{b}^+K}(\boldsymbol{r})\right)^+ \Psi(E, \boldsymbol{r}) = 0 \tag{65}$$

subtract equation (65) from equation (64) and integrate the result over the reaction volume $\mathcal{V}$, obtaining

$$[E_{\mathbf{b}K} - E]\langle \Phi_{\mathbf{b}^+K} | \Psi \rangle = \langle \Phi_{\mathbf{b}^+K} | \hat{\mathcal{L}}_{\mathbf{b}}\Psi \rangle \tag{66}$$

† It is possible that this assumption restricts a class of admissible matrices **b**. Therefore henceforth we assume that **b** is such that the assumption is satisfied.

whence

$$\Psi(E,\boldsymbol{r}) = \sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r}) \frac{\langle \Phi_{\mathbf{b}^+K} | \hat{\mathcal{L}}_{\mathbf{b}} \Psi \rangle}{E_{\mathbf{b}K} - E} \qquad \text{in } \mathcal{V} \setminus \mathcal{S} \tag{67}$$

and, because of the continuity of Ψ,

$$\Psi(E,\boldsymbol{\rho}) = \lim_{r\to\rho^-} \sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r}) \frac{\langle \Phi_{\mathbf{b}^+K} | \hat{\mathcal{L}}_{\mathbf{b}} \Psi \rangle}{E_{\mathbf{b}K} - E} \qquad \text{on } \mathcal{S}. \tag{68}$$

Projecting this equation onto the channel matrices $\boldsymbol{\Theta}$ and $\widetilde{\boldsymbol{\Theta}}$ and performing the integration in the numerator, we obtain for $r < \rho$

$$\mathbf{P}(E,r) = \frac{\hbar^2}{2m\rho} \sum_K \frac{\mathbf{F}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E} \left[\left(\frac{2m\rho c}{\hbar} \right) \mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho) \right] \tag{69}$$

$$\mathbf{Q}(E,r) = \frac{\hbar^2}{2m\rho} \sum_K \frac{\mathbf{G}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E} \left[\left(\frac{2m\rho c}{\hbar} \right) \mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho) \right] \tag{70}$$

and for $r = \rho$

$$\mathbf{P}(E,\rho) = \frac{\hbar^2}{2m\rho} \lim_{r\to\rho^-} \sum_K \frac{\mathbf{F}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E} \left[\left(\frac{2m\rho c}{\hbar} \right) \mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho) \right] \tag{71}$$

$$\mathbf{Q}(E,\rho) = \frac{\hbar^2}{2m\rho} \lim_{r\to\rho^-} \sum_K \frac{\mathbf{G}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E} \left[\left(\frac{2m\rho c}{\hbar} \right) \mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho) \right]. \tag{72}$$

Next, we define the matrix $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$ as

$$\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho) = \frac{\hbar^2}{2m\rho} \lim_{r\to\rho^-} \sum_K \frac{\left[\rho \int_{4\pi} \mathrm{d}^2\boldsymbol{n}\boldsymbol{\Theta}^+(\boldsymbol{n})\Phi_{\mathbf{b}K}(\boldsymbol{r})\right]\left[\rho \int_{4\pi} \mathrm{d}^2\boldsymbol{n}'\Phi^+_{\mathbf{b}^+K}(\boldsymbol{\rho}')\boldsymbol{\Theta}(\boldsymbol{n}')\right]}{E_{\mathbf{b}K} - E}. \tag{73}$$

After performing the integrations, equation (73) simplifies to the form

$$\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho) = \frac{\hbar^2}{2m\rho} \lim_{r\to\rho^-} \sum_K \frac{\mathbf{F}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E}. \tag{74}$$

Comparing equations (71) and (74) we obtain the following relation between the large and small components of the radial functions in different channels

$$\mathbf{P}(E,\rho) = \boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho) \left[\left(\frac{2m\rho c}{\hbar} \right) \mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho) \right]. \tag{75}$$

On substituting this equation to equation (14) we obtain the relation between the matrices $\boldsymbol{\mathcal{R}}(E,\rho)$, $\mathbf{b}$ and $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$

$$\boldsymbol{\mathcal{R}}^{-1}(E,\rho) = \mathbf{b} + \boldsymbol{\mathcal{R}}^{-1}_{\mathbf{b}}(E,\rho) \tag{76}$$

which implies $\boldsymbol{\mathcal{R}}(E,\rho) = \boldsymbol{\mathcal{R}}_{\mathbf{0}}(E,\rho)$. Moreover, in virtue of Hermicity of the matrix $\boldsymbol{\mathcal{R}}(E,\rho)$ we have

$$\boldsymbol{\mathcal{R}}^+_{\mathbf{b}}(E,\rho) = \boldsymbol{\mathcal{R}}_{\mathbf{b}^+}(E,\rho). \tag{77}$$

Once the matrix $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$ has been found, one may use equations (76) and (38) to obtain the scattering matrix $\mathbf{S}(E)$. Another possibility is to use directly the equation

$$\begin{aligned}\mathbf{S}(E) = {} & \boldsymbol{\mathcal{O}}^{-1}(E,\rho)\left\{\mathbf{I} - \boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)\left[\mathbf{L}(E,\rho) - \mathbf{b}\right]\right\}^{-1}\left\{\mathbf{I} - \boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)\left[\mathbf{L}^+(E,\rho) - \mathbf{b}\right]\right\}\boldsymbol{\mathcal{I}}(E,\rho) \\ = {} & \boldsymbol{\mathcal{I}}(E,\rho)\left\{\mathbf{I} - \left[\mathbf{L}^+(E,\rho) - \mathbf{b}\right]\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)\right\} \\ & \times \left\{\mathbf{I} - \left[\mathbf{L}(E,\rho) - \mathbf{b}\right]\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)\right\}^{-1}\boldsymbol{\mathcal{O}}^{-1}(E,\rho)\end{aligned} \tag{78}$$

which may be obtained from equation (38) after simple manipulations.

The goal of our further considerations will be to find a tractable form of $\mathcal{R}_{\mathbf{b}}(E,\rho)$. At first we shall show that the operations $\lim_{r\to\rho^-}$ and $\sum_K$ in equations (68) and (71)–(74) in general do *not* commute. This fact was not recognized before and was a source of errors in previous presentations of the Wigner R-matrix theory for systems described by the Dirac equation [3, 4]. We introduce a new function

$$\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r}) = \Theta(\boldsymbol{n})\frac{\overline{\mathbf{P}}_{\mathbf{b}}(E,r)}{r} + \widetilde{\Theta}(\boldsymbol{n})\frac{\overline{\mathbf{Q}}_{\mathbf{b}}(E,r)}{r} \tag{79}$$

defined by the eigenfunction expansion

$$\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r}) = \sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})\frac{\langle\Phi_{\mathbf{b}^+K}|\hat{\mathcal{L}}_{\mathbf{b}}\Psi\rangle}{E_{\mathbf{b}K}-E} \tag{80}$$

in the *whole* reaction volume $\mathcal{V}$ *including* the surface $\mathcal{S}$. In particular,

$$\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{\rho}) = \sum_K \Phi_{\mathbf{b}K}(\boldsymbol{\rho})\frac{\langle\Phi_{\mathbf{b}^+K}|\hat{\mathcal{L}}_{\mathbf{b}}\Psi\rangle}{E_{\mathbf{b}K}-E} \qquad \text{on } \mathcal{S}. \tag{81}$$

Therefore, from equations (67) and (80) we have

$$\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r}) = \Psi(E,\boldsymbol{r}) \qquad \text{in } \mathcal{V}\setminus\mathcal{S} \tag{82}$$

but equations (50) and (81) imply

$$\hat{\mathcal{L}}_{\mathbf{b}}\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{\rho}) = 0 \qquad \text{on } \mathcal{S}. \tag{83}$$

The difference

$$\chi_{\mathbf{b}}(E,\boldsymbol{r}) = \Psi(E,\boldsymbol{r}) - \overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r}) \tag{84}$$

is the Kapur–Peierls function for the problem under consideration. Equation (82) shows that it vanishes identically in the interior of the reaction volume. Projection of equations (80) and (81) onto the channel matrices gives for $r<\rho$

$$\overline{\mathbf{P}}_{\mathbf{b}}(E,r) = \frac{\hbar^2}{2m\rho}\sum_K \frac{\mathbf{F}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K}-E}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho)\right] \tag{85}$$

$$\overline{\mathbf{Q}}_{\mathbf{b}}(E,r) = \frac{\hbar^2}{2m\rho}\sum_K \frac{\mathbf{G}_{\mathbf{b}K}(r)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K}-E}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho)\right] \tag{86}$$

and for $r=\rho$

$$\overline{\mathbf{P}}_{\mathbf{b}}(E,\rho) = \frac{\hbar^2}{2m\rho}\sum_K \frac{\mathbf{F}_{\mathbf{b}K}(\rho)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K}-E}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho)\right] \tag{87}$$

$$\overline{\mathbf{Q}}_{\mathbf{b}}(E,\rho) = \frac{\hbar^2}{2m\rho}\sum_K \frac{\mathbf{G}_{\mathbf{b}K}(\rho)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K}-E}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho) - \mathbf{b}\mathbf{P}(E,\rho)\right]. \tag{88}$$

Equations (85)–(88) are to be compared with equations (69)–(72). Obviously, we have

$$\overline{\mathbf{P}}_{\mathbf{b}}(E,r) = \mathbf{P}(E,r) \qquad \overline{\mathbf{Q}}_{\mathbf{b}}(E,r) = \mathbf{Q}(E,r) \qquad \text{for } r<\rho \tag{89}$$

but

$$-\frac{\hbar^2}{2m\rho}\mathbf{b}\overline{\mathbf{P}}_{\mathbf{b}}(E,\rho) + c\hbar\overline{\mathbf{Q}}_{\mathbf{b}}(E,\rho) = \mathbf{0} \qquad \text{at } r=\rho. \tag{90}$$

In the next step, we define the matrix $\mathbf{R}_{\mathbf{b}}(E,\rho)$ by the relation

$$\mathbf{R}_{\mathbf{b}}(E,\rho)=\frac{\hbar^2}{2m\rho}\sum_K\frac{\left[\rho\int_{4\pi}\mathrm{d}^2\boldsymbol{n}\boldsymbol{\Theta}^+(\boldsymbol{n})\Phi_{\mathbf{b}K}(\boldsymbol{\rho})\right]\left[\rho\int_{4\pi}\mathrm{d}^2\boldsymbol{n}'\Phi^+_{\mathbf{b}^+K}(\boldsymbol{\rho}')\boldsymbol{\Theta}(\boldsymbol{n}')\right]}{E_{\mathbf{b}K}-E} \tag{91}$$

which may be reduced to the form

$$\mathbf{R}_{\mathbf{b}}(E,\rho)=\frac{\hbar^2}{2m\rho}\sum_K\frac{\mathbf{F}_{\mathbf{b}K}(\rho)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K}-E}. \tag{92}$$

From equations (87) and (92) it is seen that the matrix $\mathbf{R}_{\mathbf{b}}(E,\rho)$ relates $\overline{\mathbf{P}}_{\mathbf{b}}(E,\rho)$ to $\mathbf{P}(E,\rho)$ and $\mathbf{Q}(E,\rho)$ according to the formula

$$\overline{\mathbf{P}}_{\mathbf{b}}(E,\rho)=\mathbf{R}_{\mathbf{b}}(E,\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right]. \tag{93}$$

Note the difference between equations (71), (73)–(75) and equations (87), (91)–(93) defining the matrices $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$ and $\mathbf{R}_{\mathbf{b}}(E,\rho)$, respectively.

To find the relation between the matrices $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$ and $\mathbf{R}_{\mathbf{b}}(E,\rho)$, we derive a differential equation satisfied by the function $\overline{\Psi}_{\mathbf{b}}$ in the reaction volume $\mathcal{V}$. Acting on both sides of equation (80) with the operator $\hat{\mathcal{H}}_{\mathbf{b}}-E$ and utilizing equations (56) and (83), we get

$$\left[\hat{H}-E\right]\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r})=\sum_K\Phi_{\mathbf{b}K}(\boldsymbol{r})\langle\Phi_{\mathbf{b}^+K}|\hat{\mathcal{L}}_{\mathbf{b}}\Psi\rangle. \tag{94}$$

By virtue of equation (60) the above equation may be further transformed to the form

$$\begin{aligned}\left[\hat{H}-E\right]\overline{\Psi}_{\mathbf{b}}(E,\boldsymbol{r})=\frac{\hbar^2}{2m\rho}\frac{\delta(r-\rho)}{\rho}&\left[\boldsymbol{\Theta}(\boldsymbol{n})+\left(\frac{\hbar}{2m\rho c}\right)\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\mathbf{b}\right]\\&\times\mathbf{A}_{\mathbf{b}}(\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right].\end{aligned} \tag{95}$$

Then, projecting equation (95) onto the channel matrices $\boldsymbol{\Theta}$ and $\widetilde{\boldsymbol{\Theta}}$ we find

$$\begin{aligned}&-c\hbar\left[\frac{\mathrm{d}\overline{\mathbf{Q}}_{\mathbf{b}}(E,r)}{\mathrm{d}r}-\frac{\mathcal{K}}{r}\overline{\mathbf{Q}}_{\mathbf{b}}(E,r)\right]+\left[(mc^2-E)\mathbf{I}+\mathbf{V}(r)\right]\overline{\mathbf{P}}_{\mathbf{b}}(E,r)\\&\qquad=c\hbar\left(\frac{\hbar}{2m\rho c}\right)\delta(r-\rho)\mathbf{A}_{\mathbf{b}}(\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right]\end{aligned} \tag{96}$$

$$\begin{aligned}&c\hbar\left[\frac{\mathrm{d}\overline{\mathbf{P}}_{\mathbf{b}}(E,r)}{\mathrm{d}r}+\frac{\mathcal{K}}{r}\overline{\mathbf{P}}_{\mathbf{b}}(E,r)\right]+\left[\left(-mc^2-E\right)\mathbf{I}+\mathbf{V}(r)\right]\overline{\mathbf{Q}}_{\mathbf{b}}(E,r)\\&\qquad=c\hbar\left(\frac{\hbar}{2m\rho c}\right)^2\delta(r-\rho)\mathbf{b}\mathbf{A}_{\mathbf{b}}(\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right].\end{aligned} \tag{97}$$

Integration of both sides of equations (96) and (97) over the interval $\rho-\varepsilon\leqslant r\leqslant\rho$, $(\varepsilon\to 0^+)$, gives

$$-c\hbar\left[\overline{\mathbf{Q}}_{\mathbf{b}}(E,\rho)-\mathbf{Q}(E,\rho)\right]=c\hbar\left(\frac{\hbar}{2m\rho c}\right)\mathbf{A}_{\mathbf{b}}(\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right] \tag{98}$$

$$c\hbar\left[\overline{\mathbf{P}}_{\mathbf{b}}(E,\rho)-\mathbf{P}(E,\rho)\right]=c\hbar\left(\frac{\hbar}{2m\rho c}\right)^2\mathbf{b}\mathbf{A}_{\mathbf{b}}(\rho)\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho)-\mathbf{b}\mathbf{P}(E,\rho)\right] \tag{99}$$

which together with equation (90) constitute a set of algebraic equations for the square matrix $\mathbf{A_b}(\rho)$ and the column matrices $\overline{\mathbf{P}}_\mathbf{b}(E,\rho)$ and $\overline{\mathbf{Q}}_\mathbf{b}(E,\rho)$. The solution to this system is

$$\mathbf{A_b}(\rho) = \frac{(2m\rho c/\hbar)^2\mathbf{I}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}} \tag{100}$$

$$\overline{\mathbf{P}}_\mathbf{b}(E,\rho) = \frac{(2m\rho c/\hbar)\mathbf{I}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{P}(E,\rho) + \mathbf{bQ}(E,\rho)\right] \tag{101}$$

$$\overline{\mathbf{Q}}_\mathbf{b}(E,\rho) = \frac{\mathbf{b}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}}\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{P}(E,\rho) + \mathbf{bQ}(E,\rho)\right] \tag{102}$$

provided the matrix $\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}$ is non-singular. From equations (75), (93) and (101), after simple transformations, we obtain the desired relation between the matrices $\boldsymbol{\mathcal{R}}_\mathbf{b}(E,\rho)$ and $\mathbf{R_b}(E,\rho)$

$$\boldsymbol{\mathcal{R}}_\mathbf{b}(E,\rho) = \mathbf{R_b}(E,\rho) - \frac{\mathbf{b}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}} \tag{103}$$

and the explicit form of the matrix $\boldsymbol{\mathcal{R}}_\mathbf{b}(E,\rho)$

$$\boldsymbol{\mathcal{R}}_\mathbf{b}(E,\rho) = \frac{\hbar^2}{2m\rho}\sum_K \frac{\mathbf{F}_{\mathbf{b}K}(\rho)\mathbf{F}^+_{\mathbf{b}^+K}(\rho)}{E_{\mathbf{b}K} - E} - \frac{\mathbf{b}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}}. \tag{104}$$

This result shows that indeed in the relativistic case the operations $\lim_{r\to\rho^-}$ and $\sum_K$ in equations (68) and (71)–(74) in general do not commute. An analytically solvable example illustrating this phenomenon has been presented in [20] appendix B. We note also that in the non-relativistic limit the difference $\boldsymbol{\mathcal{R}}_\mathbf{b}(E,\rho) - \mathbf{R_b}(E,\rho)$ vanishes.

Another result following from the above considerations is an explicit form of the Kapur–Peierls function $\chi_\mathbf{b}(E,\boldsymbol{r})$. From equation (82) we have

$$\chi_\mathbf{b}(E,\boldsymbol{r}) \equiv 0 \qquad \text{in } \mathcal{V}\setminus\mathcal{S} \tag{105}$$

the result already stated earlier, while equations (84) and (98)–(100) give

$$\chi_\mathbf{b}(E,\boldsymbol{\rho}) = -\frac{1}{\rho}\left[\boldsymbol{\Theta}(\boldsymbol{n})\mathbf{b} - \left(\frac{2m\rho c}{\hbar}\right)\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\right]\frac{\mathbf{I}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}} \times\left[\left(\frac{2m\rho c}{\hbar}\right)\mathbf{Q}(E,\rho) - \mathbf{bP}(E,\rho)\right] \qquad \text{on } \mathcal{S}. \tag{106}$$

We observe that in general $\chi_\mathbf{b}(E,\boldsymbol{\rho}) \neq 0$, i.e. $\overline{\mathbf{P}}_\mathbf{b}(E,\rho) \neq \mathbf{P}(E,\rho)$ and $\overline{\mathbf{Q}}_\mathbf{b}(E,\rho) \neq \mathbf{Q}(E,\rho)$. There is, however, an exceptional case when for a given energy E the equalities $\overline{\mathbf{P}}_\mathbf{b}(E,\rho) = \mathbf{P}(E,\rho)$ and $\overline{\mathbf{Q}}_\mathbf{b}(E,\rho) = \mathbf{Q}(E,\rho)$ hold simultaneously. This happens if and only if $\mathbf{b} = \boldsymbol{\mathcal{R}}^{-1}(E,\rho)$. In such a case the energy E coincides with one of the eigenvalues, say $E_{\mathbf{b}K}$, of the extended Hamiltonian $\hat{\mathcal{H}}_\mathbf{b}$ and $\Psi = \overline{\Psi}_\mathbf{b} = \Phi_{\mathbf{b}K}$.

Equation (100) allows us to rewrite equation (60), the 'incompleteness' relation on the surface $\mathcal{S}$, in the form

$$\sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})\Phi^+_{\mathbf{b}^+K}(\boldsymbol{\rho}') = \frac{\delta(r-\rho)}{\rho^2}\left[\boldsymbol{\Theta}(\boldsymbol{n}) + \left(\frac{\hbar}{2m\rho c}\right)\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\mathbf{b}\right]\frac{(2m\rho c/\hbar)^2\mathbf{I}}{\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I}} \times\left[\boldsymbol{\Theta}^+(\boldsymbol{n}') + \left(\frac{\hbar}{2m\rho c}\right)\mathbf{b}\widetilde{\boldsymbol{\Theta}}^+(\boldsymbol{n}')\right]. \tag{107}$$

Two limiting cases may be considered. If $\mathbf{b} = \mathbf{0}$ (in other words, if the functions $\mathbf{G}_{\mathbf{b}K}$ are forced to vanish at $r = \rho$), then equations (48) and (107) show that the set $\{\Phi_{\mathbf{0}K}\}$ is complete on $\mathcal{S}$ in the subspace of *upper* components

$$\sum_K \Phi_{\mathbf{0}K}(\boldsymbol{r})\Phi^+_{\mathbf{0}K}(\boldsymbol{\rho}') = \delta(\boldsymbol{r}-\boldsymbol{\rho}')\frac{1+\beta}{2}. \tag{108}$$

In this case from equations (101) and (102) we have $\overline{\mathbf{P}}_{\mathbf{0}}(E,\rho) = \mathbf{P}(E,\rho)$ and $\overline{\mathbf{Q}}_{\mathbf{0}}(E,\rho) = \mathbf{0}$ and consequently

$$\frac{1+\beta}{2}\overline{\Psi}_{\mathbf{0}}(E,\rho) = \frac{1+\beta}{2}\Psi(E,\rho) \qquad \frac{1-\beta}{2}\overline{\Psi}_{\mathbf{0}}(E,\rho) = 0. \tag{109}$$

In turn, if $\mathbf{b} = \mp\infty$ (i.e. if $\mathbf{F}_{\mathbf{b}K}(\rho) = \mathbf{0}$), then equations (49) and (107) imply

$$\sum_K \Phi_{\mp\infty K}(\boldsymbol{r})\Phi^+_{\mp\infty K}(\boldsymbol{\rho}') = \delta(\boldsymbol{r}-\boldsymbol{\rho}')\frac{1-\beta}{2} \tag{110}$$

i.e. the set $\{\Phi_{\mp\infty K}\}$ is complete on $\mathcal{S}$ in the subspace of *lower* components. In this case we have $\overline{\mathbf{Q}}_{\mp\infty}(E,\rho) = \mathbf{Q}(E,\rho)$ and $\overline{\mathbf{P}}_{\mp\infty}(E,\rho) = \mathbf{0}$ hence

$$\frac{1-\beta}{2}\overline{\Psi}_{\mp\infty}(E,\rho) = \frac{1-\beta}{2}\Psi(E,\rho) \qquad \frac{1+\beta}{2}\overline{\Psi}_{\mp\infty}(E,\rho) = 0. \tag{111}$$

Finally, we observe that if in equation (107) the speed of light c approaches infinity, we obtain the relation

$$\sum_K \Phi_{\mathbf{b}K}(\boldsymbol{r})\Phi^+_{\mathbf{b}^+K}(\boldsymbol{\rho}') = \delta(\boldsymbol{r}-\boldsymbol{\rho}')\frac{1+\beta}{2}. \tag{112}$$

This relation looks similar to equation (108) but differs from the latter because now elements of the matrix $\mathbf{b}$ may be arbitrary (although finite) and the lower components of the functions $\{\Phi_{\mathbf{b}K}\}$ and $\{\Phi_{\mathbf{b}^+K}\}$ vanish identically. Equation (112) shows that in the non-relativistic limit the basis set generated by the boundary-value problem in the interior of the reaction volume $\mathcal{V}$ is also complete on the boundary $\mathcal{S}$, irrespective of values of matrix elements of the matrix $\mathbf{b}$, as long as the latter are finite. This explains why the construction of the R-matrix theories for the Schrödinger equation does not encounter any difficulties. It is a simple task to obtain non-relativistic limits of all formulae derived above and to verify that they coincide with corresponding well known non-relativistic expressions provided one defines a matrix of the non-relativistic boundary condition constants $\mathbf{b}_{\mathrm{N}} = \mathbf{b} - \boldsymbol{\mathcal{K}}$ [20]. In particular one finds that in the non-relativistic limit, the Kapur–Peierls function $\chi_{\mathbf{b}}$ vanishes on the reaction surface but has there a non-vanishing normal derivative which agrees with the result of Kapur and Peierls [1].

5. Discussion

We are now prepared to obtain the relativistic generalizations of the Wigner and Kapur–Peierls theories. Both theories are particular cases of the general approach exposed in sections 3 and 4. In the Wigner theory the matrix $\mathbf{b}$ is taken to be Hermitian†, $\mathbf{b}^+ = \mathbf{b}$, which gives

$$\hat{\mathcal{H}}^+_{\mathbf{b}} = \hat{\mathcal{H}}_{\mathbf{b}} \qquad \Phi^{\perp}_{\mathbf{b}K}(E,\boldsymbol{r}) = \Phi_{\mathbf{b}K}(E,\boldsymbol{r}) \qquad E^*_{\mathbf{b}K} = E_{\mathbf{b}K} \tag{113}$$

† In practically all papers on the Wigner R-matrix theory the matrix $\mathbf{b}$ was chosen to be real and diagonal as suggested by Teichmann T and Wigner E P 1952 *Phys. Rev.* **87** 123. Although this restriction may simplify some applications, it is not necessary and an application of the R-matrix theory with non-diagonal $\mathbf{b}$ was presented by Zvijac D J, Heller E J and Light J C 1975 *J. Phys. B: At. Mol. Phys.* **8** 1016, section 5.

and

$$\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)=\frac{\bar{h}^2}{2m\rho}\sum_K\frac{\mathbf{F}_{\mathbf{b}K}(\rho)\mathbf{F}^{+}_{\mathbf{b}K}(\rho)}{E_{\mathbf{b}K}-E}-\frac{\mathbf{b}}{\mathbf{b}^2+(2m\rho c/\bar{h})^2\mathbf{I}}. \tag{114}$$

The scattering matrix $\mathbf{S}(E)$ may now be obtained using equations (78) and (114).

In the Kapur–Peierls theory, the matrix $\mathbf{b}$ is chosen in such a way that the Bloch operator $\hat{\mathcal{L}}_{\mathbf{b}}$, when acting on the wavefunction Ψ of the scattered particle, cancels its outgoing part on the reaction surface $\mathcal{S}$. In other words, the expression

$$\begin{aligned}\hat{\mathcal{L}}_{\mathbf{b}}\Psi(E,\boldsymbol{\rho})=\eta\frac{\delta(r-\rho)}{\rho}\boldsymbol{\Theta}(\boldsymbol{n})\left[-\frac{\bar{h}^2}{2m\rho}\mathbf{bP}(E,\rho)+c\bar{h}\mathbf{Q}(E,\rho)\right]\\ +(1-\eta)\frac{\delta(r-\rho)}{\rho}\widetilde{\boldsymbol{\Theta}}(\boldsymbol{n})\left[2m\rho c^2\mathbf{b}^{-1}\mathbf{Q}(E,\rho)-c\bar{h}\mathbf{P}(E,\rho)\right]\end{aligned} \tag{115}$$

cannot contain terms proportional to $\exp(+\mathrm{i}k\rho)$. Referring to equations (31) and (32) we find that this condition will be satisfied if the matrix $\mathbf{b}$ is

$$\mathbf{b}=\mathbf{L}(E,\rho) \tag{116}$$

where the diagonal matrix $\mathbf{L}(E,\rho)$ has been defined by equation (39). With this choice of $\mathbf{b}$ the terms $\boldsymbol{\mathcal{R}}_{\mathbf{b}}\left[\mathbf{L}-\mathbf{b}\right]$ and $\left[\mathbf{L}-\mathbf{b}\right]\boldsymbol{\mathcal{R}}_{\mathbf{b}}$ in equation (78) vanish and we get

$$\mathbf{S}(E)=\boldsymbol{\mathcal{O}}^{-1}(E,\rho)\boldsymbol{\mathcal{I}}(E,\rho)+2\mathrm{i}\epsilon\left(\frac{2m\rho c}{\bar{h}}\right)\sqrt{\frac{E-mc^2}{E+mc^2}}\boldsymbol{\mathcal{O}}^{-1}(E,\rho)\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)\boldsymbol{\mathcal{O}}^{-1}(E,\rho) \tag{117}$$

with $\boldsymbol{\mathcal{R}}_{\mathbf{b}}(E,\rho)$ given by equation (104) and $\mathbf{b}$ by equation (116). Equation (117) is the relativistic generalization of the famous Kapur–Peierls formula [1].

Next, we assume an attitude towards the papers of Rosenthal [17] and Halderson [19]. There are several errors in [17]. The function $\psi_\lambda^{(-)}$ defined by Rosenthal is an eigenfunction of the operator $-\beta(\boldsymbol{\Sigma}\cdot\boldsymbol{L}+1)$ belonging to the eigenvalue $-\kappa$ and *not* κ as he asserted†. The introduction of $\psi_\lambda^{(-)}$ is needless and misleading: for a given pair κm, *all* solutions, irrespective of whether they belong to positive or negative energies, are of the form $\psi_\lambda^{(+)}$. Therefore, in [17] all functions $\psi_\lambda^{(-)}$ should be removed and all superscripts $(+)$ should be omitted. Next, if one truncates the basis $\{\psi_\lambda\}$ to positive energy functions, as Rosenthal did, it is obvious that such a set cannot be complete anywhere. If one uses a set containing functions belonging to positive *and* negative energies (see above), then such a set must be complete for $r<\rho$ since it has been generated by a Hermitian boundary-value problem. Rosenthal's observation that the basis (including positive *and* negative energy eigenfunctions) was incomplete *on the reaction surface* was correct but his conclusion that this made derivation of the R-matrix theory for the Dirac equation impossible was wrong. We have shown above, by construction, that such a theory does exist. In spite of the errors and the incorrect conclusion Rosenthal's finding about the incompleteness of the relativistic basis set on the reaction surface should be appreciated, however.

Halderson [19] attempted to prove that the R-matrix theory was applicable to the Dirac equation, but he derived the theory only for the specific case $\mathbf{b}=\mathbf{0}$. Moreover, comparison of the argumentation used in [19] with the proof presented here shows that even in this case Halderson's proof was non-rigorous because that author assumed the completeness

† Notice that Rosenthal's definition of κ, the first unnumbered equation following equation (2) of [17], is incorrect since a matrix factor $-\beta$ is missing; this results in disagreement with relations between κ, l and $\bar{l}$ given below the second unnumbered equation of that paper.

of the basis on the surface in the subspace of upper components without proving it. In particular, interchange of the operations $\lim_{r\to a_c}$ and $\sum_\lambda$ which he admitted when arriving to equation (13) of his paper, although exceptionally possible in the very specific case discussed in that paper, was just a source of errors in previous relativistic generalizations of the Wigner theory to more general boundary conditions [3, 4]. It is clear from the context and from errors† occurring in the paragraph preceding equation (13) of [19] that Halderson was not aware of exceptionality of this case.

Finally, the following remark may be useful. It should be emphasized that the source of the term $-\mathbf{b}/(\mathbf{b}^2 + (2m\rho c/\hbar)^2\mathbf{I})$ appearing in equations (103), (104) and (114) is different from the source of the Buttle correction [27] used in applications of the R-matrix theory. In applications one must always work with *finite* sets of functions. Truncating the R-matrix basis one obtains the set which is incomplete in the *reaction volume* and to compensate the error introduced in the R-matrix expansion by the truncation one uses the Buttle correction. The term derived in the present paper is due to the incompleteness of the *infinite* relativistic R-matrix basis on the *reaction surface*. This phenomenon does not occur (cf equation (112)) in the non-relativistic theory.

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† First, for a continuous potential the derivative of G is continuous since G and F satisfy coupled first-order differential equations with continuous coefficients. For the boundary condition considered by Halderson, this is the derivative of the *eigenfunction expansion* of G which is discontinuous at $r = a_c$. Second, *both* functions G and F must be continuous for potentials finite at $r = a_c$ (but not necessarily their eigenfunction expansions). Third, one can expand a solution to the Dirac equation in a basis defined by *any* linear boundary condition of the form $\alpha G_\lambda(a_c) + \beta F_\lambda(a_c) = 0$, where α and β are two arbitrary constants such that $\alpha^2 + \beta^2 \neq 0$. However, this expansion does not converge at $r = a_c$, at least in one component; it is the goal of the present paper to show how to deal with this difficulty.

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