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Relativistic theory of photoionization of one-electron systems: an eigenchannel R -matrix approach

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Abstract

A theoretical background of an eigenchannel R -matrix approach to photoionization of relativistic one-electron systems is outlined.

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1. Introduction

A nonrelativistic eigenchannel R -matrix approach to atomic processes was proposed nearly 30 years ago (Fano and Lee, 1973; Lee, 1974). Since then, the method has evolved into one of the most powerful tools used in theoretical description of photoionization and Rydberg spectra of atoms and molecules (Greene, 1988; Hamacher, 1990; Aymar et al., 1996). A relativistic variant of the method was proposed more than a decade ago by Hamacher and Hinze (1991) and subsequently developed mathematically by Szmytkowski (1998a, 1999, 2001a, b) within the framework of the integral operators formulation of the R -matrix theory (Szmytkowski, 1998b, 1999).

The present paper is the first step towards a practical application of the relativistic eigenchannel R -matrix method in atomic physics. On the following pages we adapt the general mathematical formalism presented by us earlier (Szmytkowski, 1998a, 1999, 2001a, b) to a theoretical description of photoionization of relativistic one-electron systems.

2. Differential cross section for photoionization

Consider a Dirac electron bound in a known stationary state:

$$\Psi^{(0)}(\mathbf{r}, t) = \psi^{(0)}(\mathbf{r})e^{-i\omega^{(0)}t} \quad (1)$$

of total energy $E^{(0)} = \hbar\omega^{(0)}$. The function $\psi^{(0)}(\mathbf{r})$ is the solution of the time-independent Dirac equation

$$[\hat{\mathcal{H}}^{(0)} - E^{(0)}]\psi^{(0)}(\mathbf{r}) = 0, \quad (2)$$

with the Hamiltonian

$$\hat{\mathcal{H}}^{(0)} = -i\hbar\boldsymbol{\alpha} \cdot \nabla + \beta mc^2 + \hat{V} - \frac{Ze^2}{r}. \quad (3)$$

Here, $\boldsymbol{\alpha}$ and β are the standard Dirac matrices, while \hat{V} is a Hermitian short-range potential operator, possibly non-local and non-central.

The differential cross section for photoionization of the electron from the state (1), by a classical electromagnetic monochromatic plane wave characterized by a wave vector $\boldsymbol{\kappa}$, a polarization vector $\boldsymbol{\varepsilon}$ and frequency ω , to a state of definite spin polarization, is given by

$$\frac{d\sigma}{d\Omega} = \frac{(E + mc^2)\alpha k}{4\pi\hbar\omega} \left| \int_{\mathbb{R}^3} d^3\mathbf{r} \psi^\dagger(\mathbf{k}, \mathbf{r}) \boldsymbol{\alpha} \cdot \boldsymbol{\varepsilon} e^{i\boldsymbol{\kappa} \cdot \mathbf{r}} \psi^{(0)}(\mathbf{r}) \right|^2. \quad (4)$$

In Eq. (4) $E = E^{(0)} + \hbar\omega$ is the total energy of the ejected photoelectron, \mathbf{k} is its wave vector (with $k = |\mathbf{k}|$ defined

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in terms of E in Eq. (A.6)) while α (not to be confused with the Dirac matrix α) is the fine-structure constant. The so-called ‘final state’ function $\psi(\mathbf{k}, \mathbf{r})$ obeys the Dirac equation

$$[\hat{\mathcal{H}}^{(0)} - E]\psi(\mathbf{k}, \mathbf{r}) = 0 \quad (5)$$

with an asymptotic boundary condition

$$\psi(\mathbf{k}, \mathbf{r}) \xrightarrow{r \rightarrow \infty} \psi^C(\mathbf{k}, \mathbf{r}) + \mathcal{A}(\mathbf{n}_k, \mathbf{n}_r) \frac{e^{-i(kr + \eta \ln 2kr)}}{r}, \quad (6)$$

where

$$\psi^C(\mathbf{k}, \mathbf{r}) = \sum_{\chi m} 4\pi k^{-1} i^l e^{-i\delta_\chi^C} \psi_{\chi m}^M(\mathbf{r}) \Omega_{\chi m}^\dagger(\mathbf{n}_k) \chi. \quad (7)$$

Here, $\mathbf{n}_r = \mathbf{r}/r$, $\mathbf{n}_k = \mathbf{k}/k$, the numbers χ and m are combined parity and total angular momentum and total angular momentum projection quantum numbers, respectively, $l = |\chi + 1/2| - 1/2$, $\{\psi_{\chi m}^M(\mathbf{r})\}$ are the regular Dirac–Coulomb wave functions, defined by Eqs. (20) and (A.3), $\{\Omega_{\chi m}(\mathbf{n})\}$ are spherical spinors, χ is a two-component normalized spinor describing the orientation of photoelectron’s spin in its rest frame, while δ_χ^C is a Dirac–Coulomb phase shift defined in Eq. (A.14). Asymptotically, the function $\psi^C(\mathbf{k}, \mathbf{r})$ is a superposition of a Coulomb-modified Dirac plane wave, propagating in the direction \mathbf{n}_k , and a radially incoming, angularly modulated, spherical wave.

In the following section we shall show how to find the function $\psi(\mathbf{k}, \mathbf{r})$ with the aid of the relativistic eigenchannel R -matrix method.

3. The inner and outer regions. The R -matrix

In the R -matrix method we divide the physical space into two regions, \mathcal{V} and $\mathbb{R}^3 \setminus \mathcal{V}$, separated by the reaction surface \mathcal{S} . We choose the finite inner region \mathcal{V} to be a sphere of radius ρ , centered at the source of the Coulomb field. The volume $\mathbb{R}^3 \setminus \mathcal{V}$ is the outer region. The radius ρ is to be chosen so that in the outer region the photoelectron feels the Coulomb potential only. In the rest of this work, if the point \mathbf{r} lies on the surface \mathcal{S} , we shall denote this using the symbol $\boldsymbol{\rho}$ instead of \mathbf{r} .

In the inner region the wave function $\psi(\mathbf{k}, \mathbf{r})$ may be written as the following series:

$$\psi(\mathbf{k}, \mathbf{r}) = \sum_{\nu} c_\nu \psi_\nu(E, \mathbf{r}) \quad (\mathbf{r} \in \mathcal{V}), \quad (8)$$

where $\{\psi_\nu\}$ are eigenfunctions of the spectral problem

$$[\hat{\mathcal{H}}^{(0)} - E]\psi_\nu(E, \mathbf{r}) = 0 \quad (\mathbf{r} \in \mathcal{V}), \quad (9)$$

$$[i\alpha_\perp^{(+)}(\boldsymbol{\rho}) - \gamma^{(+)} b_\nu(E) \beta^{(+)}] \psi_\nu(E, \boldsymbol{\rho}) = 0 \quad (\boldsymbol{\rho} \in \mathcal{S}). \quad (10)$$

Here the energy E is fixed at the value $E^{(0)} + \hbar\omega$, the (real) numbers $\{b_\nu(E)\}$ are eigenvalues,

$$\gamma^{(\pm)} = \pm \left(\frac{\hbar}{2mc} \right)^{\pm 1} \quad (11)$$

($\gamma^{(-)}$ will appear in Eq. (23) and in equations following it),

$$\beta^{(+)} = \frac{1}{2}(\mathcal{J} + \beta) \quad (12)$$

with \mathcal{J} denoting the unit 4×4 matrix,

$$\alpha_\perp^{(+)}(\boldsymbol{\rho}) = \beta^{(+)} \mathbf{n}(\boldsymbol{\rho}) \cdot \boldsymbol{\alpha}, \quad (13)$$

where $\mathbf{n}(\boldsymbol{\rho})$ is a unit outward vector normal to the surface \mathcal{S} at the point $\boldsymbol{\rho}$. It was shown (Szymtkowski, 1998a, 1999) that the functions $\{\psi_\nu\}$ may be chosen to be orthonormal in the sense

$$(\psi_\nu | \beta^{(+)} \psi_\mu) = \delta_{\nu\mu}, \quad (14)$$

where $(|)$ denotes the surface inner product

$$(\phi | \psi) = \oint_{\mathcal{S}} d^2 \boldsymbol{\rho} \phi^\dagger(\boldsymbol{\rho}) \psi(\boldsymbol{\rho}). \quad (15)$$

A convenient method of finding eigensolutions to system (9) and (10) is to use the equivalent variational principle

$$b(E) = \text{stat}_{\bar{\psi}} \left\{ \frac{2mc}{\hbar} \frac{(\bar{\psi} | i\alpha_\perp^{(+)} \bar{\psi})}{(\bar{\psi} | \beta^{(+)} \bar{\psi})} + \frac{2m}{\hbar^2} \frac{\langle \bar{\psi} | [\hat{\mathcal{H}}^{(0)} - E] \bar{\psi} \rangle}{(\bar{\psi} | \beta^{(+)} \bar{\psi})} \right\}, \quad (16)$$

where $\langle | \rangle$ denotes a volume inner product defined as

$$\langle \phi | \psi \rangle = \int_{\mathcal{V}} d^3 \mathbf{r} \phi^\dagger(\mathbf{r}) \psi(\mathbf{r}). \quad (17)$$

In principle, the coefficients in the expansion (8) may be found by projecting this expansion, restricted to the surface \mathcal{S} , onto $\psi_\mu^\dagger(E, \boldsymbol{\rho}) \beta^{(+)}$, and employing then Eq. (14). After replacing μ by ν in the result, this yields

$$c_\nu = (\psi_\nu | \beta^{(+)} \psi). \quad (18)$$

However, Eq. (18) may be exploited only if the function ψ is known on the reaction surface \mathcal{S} . For this purpose, we have to find it first in the outer region, making then the limiting passage $\mathbf{r} \rightarrow \boldsymbol{\rho}$.

Due to the pure Coulomb interaction in the outer region $\mathbb{R}^3 \setminus \mathcal{V}$, the function $\psi(\mathbf{k}, \mathbf{r})$ may be expanded there as

$$\begin{aligned} \psi(\mathbf{k}, \mathbf{r}) = & \sum_{\chi m} [A_{\chi m, \chi' m'} \psi_{\chi m}^M(\mathbf{r}) \\ & + B_{\chi m, \chi' m'} \psi_{\chi m}^W(\mathbf{r})] \Omega_{\chi' m'}^\dagger(\mathbf{n}_k) \chi \quad (\mathbf{r} \in \mathbb{R}^3 \setminus \mathcal{V}). \end{aligned} \quad (19)$$

In Eq. (19), $\{A_{\chi m, \chi' m'}\}$ and $\{B_{\chi m, \chi' m'}\}$, depending on k , are so far unknown coefficients which should be found. The continuum Dirac–Coulomb functions $\{\psi_{\chi m}^M \text{ or } W(\mathbf{r})\}$

are given by

$$\psi_{\chi m}^{M \text{ or } W}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{\chi}^{M \text{ or } W}(r) \Omega_{\chi m}(\mathbf{n}_r) \\ i Q_{\chi}^{M \text{ or } W}(r) \Omega_{-\chi m}(\mathbf{n}_r) \end{pmatrix}, \quad (20)$$

where $P_{\chi}^{M \text{ or } W}(r)$ and $Q_{\chi}^{M \text{ or } W}(r)$ are the continuum radial Dirac–Coulomb functions (see Appendix A for their definitions and some useful properties).

The coefficients $\{A_{\chi m, \chi' m'}\}$ can be found by analyzing an asymptotic form of Eq. (19) and comparing it with Eqs. (6) and (7). We obtain

$$A_{\chi m, \chi' m'} = 4\pi k^{-1} i^l e^{-i\delta_{\chi}^c} \delta_{\chi \chi'} \delta_{m m'}. \quad (21)$$

To find the coefficients $\{B_{\chi m, \chi' m'}\}$, let us introduce an operator $\hat{\mathcal{R}}^{(+)}(E)$, such that for any regular solution of the equation

$$[\hat{\mathcal{R}}^{(+)}(E) - E]\phi(E, \mathbf{r}) = 0 \quad (\mathbf{r} \in \mathcal{V}^-) \quad (22)$$

(notice that we consider the inner region again!) the relation

$$\beta^{(+)}\phi(E, \boldsymbol{\rho}) = -\gamma^{(-)}\hat{\mathcal{R}}^{(+)}(E)i\alpha_{\perp}^{(+)}(\boldsymbol{\rho})\phi(E, \boldsymbol{\rho}) \quad (23)$$

is satisfied on the reaction surface \mathcal{S} . Properties of $\hat{\mathcal{R}}^{(+)}(E)$ (and related operators) have been discussed extensively by Szymtkowski (1998a, b, 1999, 2001a); in particular, it has been found that the integral kernel of $\hat{\mathcal{R}}^{(+)}(E)$ has the following spectral expansion:

$$\hat{\mathcal{R}}^{(+)}(E, \boldsymbol{\rho}, \boldsymbol{\rho}') = \sum_{\nu} \beta^{(+)}\psi_{\nu}(E, \boldsymbol{\rho})b_{\nu}^{-1}(E)\psi_{\nu}^{\dagger}(E, \boldsymbol{\rho}')\beta^{(+)}, \quad (24)$$

where the numbers $\{b_{\nu}(E)\}$ and the functions $\{\psi_{\nu}\}$ (normalized as in Eq. (14)) are eigensolutions of the system (9) and (10).

In virtue of Eq. (5), it appears that Eq. (23) holds when $\psi(\mathbf{k}, \boldsymbol{\rho})$ is substituted for $\phi(E, \boldsymbol{\rho})$, i.e.

$$\beta^{(+)}\psi(\mathbf{k}, \boldsymbol{\rho}) = -\gamma^{(-)}\hat{\mathcal{R}}^{(+)}(E)i\alpha_{\perp}^{(+)}(\boldsymbol{\rho})\psi(\mathbf{k}, \boldsymbol{\rho}). \quad (25)$$

Collecting the coefficients $\{B_{\chi m, \chi' m'}\}$ into a square matrix \mathbf{B} , after substituting Eqs. (19) and (21) into Eq. (25), we obtain the algebraic linear system

$$\mathbf{WB} = \mathbf{M}. \quad (26)$$

The square matrices \mathbf{W} and \mathbf{M} with elements

$$[\mathbf{W}]_{\chi m, \chi' m'} = P_{\chi'}^W(\rho)\delta_{\chi \chi'}\delta_{m m'} + \gamma^{(-)}Q_{\chi'}^W(\rho)R_{\chi m, \chi' m'}^{(+)} \quad (27)$$

and

$$[\mathbf{M}]_{\chi m, \chi' m'} = -4\pi k^{-1} i^l e^{-i\delta_{\chi}^c} \times [P_{\chi'}^M(\rho)\delta_{\chi \chi'}\delta_{m m'} + \gamma^{(-)}Q_{\chi'}^M(\rho)R_{\chi m, \chi' m'}^{(+)}], \quad (28)$$

respectively, depend on matrix elements of the operator $\hat{\mathcal{R}}^{(+)}(E)$:

$$R_{\chi m, \chi' m'}^{(+)} = (A_{\chi m}|\hat{\mathcal{R}}^{(+)}A_{\chi' m'}), \quad (29)$$

where

$$A_{\chi m}(\mathbf{n}_{\rho}) = \begin{pmatrix} \Omega_{\chi m}(\mathbf{n}_{\rho}) \\ 0 \end{pmatrix} \quad (30)$$

with $\mathbf{n}_{\rho} = \boldsymbol{\rho}/\rho$ (notice that in the present case $\mathbf{n}_{\rho} = \mathbf{n}(\boldsymbol{\rho})$). The elements (29) form an R -matrix $\mathbf{R}^{(+)}(E)$.

Once the coefficients $\{B_{\chi m, \chi' m'}\}$ have been found, by solving the algebraic system (26), the function $\psi(\mathbf{k}, \mathbf{r})$ is known in the outer region *and*, through the limiting passage $\mathbf{r} \rightarrow \boldsymbol{\rho}$, also on the surface \mathcal{S} . Utilizing this fact in Eq. (18), we obtain

$$c_{\nu} = \sum_{\chi m} \rho^{-1} [A_{\chi m, \chi' m'} P_{\chi}^M(\rho) + B_{\chi m, \chi' m'} P_{\chi}^W(\rho)] \times (\psi_{\nu}|A_{\chi m})\Omega_{\chi' m'}^{\dagger}(\mathbf{n}_{\mathbf{k}})\zeta. \quad (31)$$

Substitution of this result into Eq. (8) yields the function $\psi(\mathbf{k}, \mathbf{r})$ in the inner region. Thus, our task of finding $\psi(\mathbf{k}, \mathbf{r})$ in the whole space \mathbb{R}^3 has been completed and the integral in Eq. (4) may be performed.

4. Conclusions and outlook

In this paper we have presented an adaptation of the relativistic eigenchannel R -matrix method (Hamacher and Hinze, 1991; Szymtkowski, 1998a, 1999, 2001b) to a theoretical description of photoionization of relativistic one-electron systems. We work on a numerical implementation of the formalism presented above and on its extension to quasi-two-electron systems.

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Appendix A. The continuum radial Dirac–Coulomb functions

The continuum radial Dirac–Coulomb functions $P_{\chi}^{M \text{ or } W}(r)$ and $Q_{\chi}^{M \text{ or } W}(r)$ used in this work are solutions to the Dirac system

$$\begin{pmatrix} (mc^2 - E)/\hbar c - \zeta/r & -d/dr + \kappa/r \\ d/dr + \kappa/r & -(mc^2 + E)/\hbar c - \zeta/r \end{pmatrix} \begin{pmatrix} P_{\chi}^{M \text{ or } W}(r) \\ Q_{\chi}^{M \text{ or } W}(r) \end{pmatrix} = 0, \quad (A.1)$$

where

$$\zeta = \alpha Z \quad (A.2)$$

(α is the fine-structure constant). For $E > mc^2$, they may be expressed in terms of the Whittaker functions of the first ($M_{\alpha, \beta}(x)$) and second ($W_{\alpha, \beta}(x)$) kinds (Magnus et al.,

1966) in the following way:

$$\begin{pmatrix} P_x^M(r) \\ Q_x^M(r) \end{pmatrix} = C_x^M \begin{pmatrix} \cos(\phi_x)[M_{-i\eta, \gamma_x-1/2}(2ikr) + \omega_M \zeta^{-1}(\alpha + \gamma_x)M_{-i\eta, \gamma_x+1/2}(2ikr)] \\ \varepsilon \sin(\phi_x)[M_{-i\eta, \gamma_x-1/2}(2ikr) + \omega_M \zeta^{-1}(\alpha - \gamma_x)M_{-i\eta, \gamma_x+1/2}(2ikr)] \end{pmatrix}, \quad (\text{A.3})$$

$$\begin{pmatrix} P_x^W(r) \\ Q_x^W(r) \end{pmatrix} = C_x^W \begin{pmatrix} W_{-i\eta, \gamma_x-1/2}(2ikr) + \omega_W W_{-i\eta, \gamma_x+1/2}(2ikr) \\ \zeta^{-1}(\alpha + \gamma_x)W_{-i\eta, \gamma_x-1/2}(2ikr) + \omega_W \zeta^{-1}(\alpha - \gamma_x)W_{-i\eta, \gamma_x+1/2}(2ikr) \end{pmatrix}, \quad (\text{A.4})$$

where

$$\gamma_x = \sqrt{\alpha^2 - \zeta^2}, \quad (\text{A.5})$$

$$k = \frac{\sqrt{(E - mc^2)(E + mc^2)}}{ch}, \quad (\text{A.6})$$

$$\varepsilon = \sqrt{\frac{E - mc^2}{E + mc^2}}, \quad (\text{A.7})$$

$$\phi_x = \arg\left(1 + i \frac{\alpha + \gamma_x}{\eta - \zeta}\right), \quad (\text{A.8})$$

$$\eta = \frac{1}{2}\zeta(\varepsilon^{-1} + \varepsilon), \quad \zeta = \frac{1}{2}\zeta(\varepsilon^{-1} - \varepsilon), \quad (\text{A.9})$$

$$\omega_M = -i\zeta^{-1} \frac{\eta\alpha + \zeta\gamma_x}{2\gamma_x(2\gamma_x + 1)}, \quad (\text{A.10})$$

$$C_x^M = \frac{|\Gamma(\gamma_x + 1 + i\eta)|}{\Gamma(2\gamma_x + 1)} \exp\left[\frac{1}{2}\pi\eta - i\frac{1}{2}\pi\gamma_x\right], \quad (\text{A.11})$$

$$\omega_W = -\frac{(\alpha + \gamma_x) + i(\eta - \zeta)}{(\alpha - \gamma_x) + i(\eta - \zeta)}, \quad (\text{A.12})$$

$$C_x^W = \frac{(\alpha - \gamma_x) + i(\eta - \zeta)}{2\gamma_x} \times \exp\left[-\frac{1}{2}\pi\eta + i\frac{1}{2}\pi(l - 1) - i\delta_x^C\right], \quad (\text{A.13})$$

$$\delta_x^C = \frac{1}{2}\pi(l + 1 - \gamma_x) - \sigma_{\gamma_x} - \phi_x, \quad (\text{A.14})$$

$$\sigma_{\gamma_x} = \arg(\gamma_x + 1 + i\eta). \quad (\text{A.15})$$

For large values of r , their asymptotic forms are:

$$\begin{pmatrix} P_x^M(r) \\ Q_x^M(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} \begin{pmatrix} \sin[kr + \eta \ln 2kr - \frac{1}{2}\pi l + \delta_x^C] \\ \varepsilon \cos[kr + \eta \ln 2kr - \frac{1}{2}\pi l + \delta_x^C] \end{pmatrix}, \quad (\text{A.16})$$

$$\begin{pmatrix} P_x^W(r) \\ Q_x^W(r) \end{pmatrix} \xrightarrow{r \rightarrow \infty} \begin{pmatrix} i \\ \varepsilon \end{pmatrix} \exp[-i(kr + \eta \ln 2kr - \frac{1}{2}\pi l + \delta_x^C)]. \quad (\text{A.17})$$

References

- Aymar, M., Greene, C.H., Luc-Koenig, E., 1996. Multichannel Rydberg spectroscopy of complex atoms. *Rev. Mod. Phys.* 68, 1015.
- Fano, U., Lee, C.M., 1973. Variational calculation of R matrices. Application to Ar photoabsorption. *Phys. Rev. Lett.* 31, 1573.
- Greene, C.H., 1988. Variational calculation of channel interaction parameters. In: Briggs, J.S., Kleinpoppen, H., Lutz, H.O. (Eds.), *Fundamental Processes of Atomic Dynamics*. Plenum, New York, pp. 105.
- Hamacher, P., 1990. Die R -Matrix-Eigenwert-Theorie. Resonanzen bei der Elektron-Atom-Streuung und der Photoionisation von Atomen. Ph. D. Thesis, Universität Bielefeld.
- Hamacher, P., Hinze, J., 1991. Finite-volume variational method for the Dirac equation. *Phys. Rev. A* 44, 1705.
- Lee, C.M., 1974. Spectroscopy and collision theory. III. Atomic eigenchannel calculation by a Hartree-Fock-Roothaan method. *Phys. Rev. A* 10, 584.
- Magnus, W., Oberhettinger, F., Soni, R.P., 1966. *Formulas and Theorems for the Special Functions of Mathematical Physics*, 3rd Edition. Springer, Berlin.
- Szymtkowski, R., 1998a. Unified construction of variational R -matrix methods for the Dirac equation. *Phys. Rev. A* 57, 4351.
- Szymtkowski, R., 1998b. Operator formulation of Wigner's R -matrix theories for the Schrödinger and Dirac equations. *J. Math. Phys.* 39, 5231 (Erratum: 1999, 40, 4181).
- Szymtkowski, R., 1999. R -matrix Method for the Schrödinger and Dirac Equations. Wydawnictwo Politechniki Gdańskiej, Gdańsk (in Polish).
- Szymtkowski, R., 2001a. Analogs of the Hellmann-Feynman theorem in the R -matrix theory. *Phys. Lett. A* 280, 105.
- Szymtkowski, R., 2001b. Variational R -matrix methods for many-electron systems: unified relativistic theory. *Phys. Rev. A* 31, 062704.