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Atoms-Photonic Field Interaction: Influence Functional and Perturbation Theory

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Additional information is available at the end of the chapter

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Abstract

We study the dynamics of one-electron atoms interacting with a pulsed, elliptically polarized, ultrashort, and coherent state. We use path integral methods. We path integrate the photonic part and extract the corresponding influence functional describing the interaction of the pulse with the atomic electron. Then we angularly decompose it. We keep the first-order angular terms in all but the last factor as otherwise their angular integration would contribute infinities as the number of time slices tends to infinity. Further we use the perturbative expansion of the last factor in powers of the inverse volume and integrate on time. Finally, we obtain a closed angularly decomposed expression of the whole path integral. As an application we develop a scattering theory and study the two-photon ionization of hydrogen.

Keywords: path integrals, influence functional, perturbation, coherent state, hydrogen, sign solved propagator, two photons

1. Introduction

The study of the interaction of radiation with matter is an area of major importance in physics. The production in laboratories of pulses of various durations and central frequencies has given a further boost in that study. These pulses can be used in the study of various elementary processes such as the excitation or photoionization of atoms [1–7]. This is possible due to their short time length of the order of a few femtoseconds or of a few hundreds attoseconds. Sub-100-as pulses have been generated as well. Moreover, their photons' energy may belong in the ultraviolet or extreme ultraviolet and therefore just one or two photons may be enough to cause excitation or ionization.

In the present chapter, we introduce a fully quantum mechanical field theoretical treatment, for the interaction of a pulsed, elliptically polarized ultrashort coherent state with one optically active electron atoms. We use path integral methods. So we integrate the photonic part and extract the corresponding influence functional describing the interaction of the pulse with the atomic electron.

Proceeding we use the discrete form of that influence functional and angularly decompose its expression. We keep first-order angular terms in all but the last factor as otherwise their angular integration would contribute infinites as the number of time slices tends to infinity. Further, we use the perturbative expansion of the last factor in powers of the inverse volume and integrate on time. So we generate a perturbative series describing the action of the photonic field on the electron of the atom. It includes photonic and vacuum fluctuations contributions. Moreover, we manipulate the angular parts of the atomic action via standard path integral methods to finally obtain a closed angularly decomposed expression of the whole path integral.

As an application we develop a scattering theory and we study the two-photon ionization of hydrogen from its ground state to continuum. For the same transitions and to the same order vacuum fluctuation terms contribute as well. In the present application we consider orthogonal pulses. We use the propagator that appears in its sign solved propagator (SSP) form Ref. [8]. Previously, we have considered other kinds of photonic states interacting with one-electron atoms (see Refs. [6, 7, 9, 10]).

The present chapter proceeds as follows. In Section 2, we describe the present system and integrate its photonic part. Then in Section 3, we give the angular decomposition of the propagator in the case of elliptic polarization. In Section 4, we give an application and our conclusions in Section 5. Finally, in the Appendix we give some functions necessary in the evaluation of certain integrals.

2. System Hamiltonian and path integration

In the present chapter, we consider a one-electron atom initially in its ground state under the action of a coherent state. Therefore, the system Hamiltonian H can be decomposed into a sum of three terms. The electron's one H_e , the photonic field one H_f , and an interaction term of the photonic field with the electron H_I . that is,

$$H = H_e + H_f + H_I. \quad (1)$$

H_e has the form

$$H_e = \frac{1}{2} \vec{p}^2 + V(\vec{r}), \quad (2)$$

where $V(\vec{r})$ is the atomic potential. The photonic field has the Hamiltonian

$$H_f = \omega a^\dagger a, \quad (3)$$

while the interaction term H_I in the Power-Zienau-Woolley formalism takes the form

$$H_I = -e\vec{r} \cdot \vec{E}_f(\vec{r}, \tau). \quad (4)$$

$\vec{E}_f(\vec{r}, \tau)$ is the field operator of the photonic pulse given by the expression

$$\vec{E}_f(\vec{r}, \tau) = \frac{1}{\sqrt{V}} i l(\omega) \wp(\tau) \left[\hat{\varepsilon} a e^{i\vec{k}_{ph} \cdot \vec{r}} - \hat{\varepsilon}^* a^\dagger e^{-i\vec{k}_{ph} \cdot \vec{r}} \right]. \quad (5)$$

$\wp(\tau)$ is the pulse's envelope function. In Eq. (5) $l(\omega) = \sqrt{2\pi\omega}$ is a real frequency function, $\hat{\varepsilon}$ is the polarization vector, ω is the pulse's carrier frequency, \vec{k}_{ph} is the radiation wave vector and V is a large volume. Then H_I has the form

$$H_I = g(\tau)a + g^*(\tau)a^\dagger. \quad (6)$$

We have set

$$g(\tau) = -\frac{1}{\sqrt{V}} i e l(\omega) \wp(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i\vec{k}_{ph} \cdot \vec{r}(\tau)}. \quad (7)$$

Now we combine the photonic field variables in the term

$$H_0(a^\dagger, a; \tau) = H_f + H_I = \omega a^\dagger a + g(\tau)a + g^*(\tau)a^\dagger. \quad (8)$$

The propagator between the initial and final states corresponding to the Hamiltonian Eq. (1) can be obtained by integrating on both the space and photonic field variables. At first we integrate the photonic field variables, which appear only in H_0 (Eq. (8)). Then we obtain the following path integral of only the spatial variables:

$$K(\alpha_f, \vec{r}_f, t_f; \alpha_i, \vec{r}_i, t_i) = \int D\vec{r}(\tau) \frac{D\vec{p}(\tau)}{(2\pi)^3} \times \exp \left[i \int_{t_i}^{t_f} d\tau \left(\vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau)) \right) - i \int_{t_i}^{t_f} d\tau g(\tau) Z(\tau, t_i) - \frac{1}{2} (|\alpha_f|^2 + |\alpha_i|^2) + Y(t_f, t_i) \alpha_f^* \alpha_i + Z(t_f, t_i) \alpha_f^* - i \alpha_i X(t_f, t_i) \right], \quad (9)$$

where $Y(t_f, t_i)$, $X(t_f, t_i)$, and $Z(t_f, t_i)$ read:

$$Y(t_f, t_i) = \exp \left[-i \int_{t_i}^{t_f} d\tau \omega(\tau) \right] = \exp \left(-i\omega(t_f - t_i) \right), \quad (10)$$

$$X(t_f, t_i) = \int_{t_i}^{t_f} d\tau g(\tau) Y(\tau, t_i), \quad (11)$$

$$Z(t_f, t_i) = -i \int_{t_i}^{t_f} d\tau g^*(\tau) \exp \left[-i \int_{\tau}^{t_f} d\tau' \omega(\tau') \right]. \quad (12)$$

The propagator in Eq. (9) with diagonal field variables ($\alpha_i = \alpha_f = \alpha$) can be written as

$$K(\alpha, \vec{r}_f, t_f; \alpha, \vec{r}_i, t_i) = \int D\vec{r}(\tau) \frac{D\vec{p}(\tau)}{(2\pi)^3} \exp \left[i \int_{t_i}^{t_f} d\tau \left[\vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau)) \right] \right. \\ \left. + A - B|\alpha|^2 + D_1\alpha + D\alpha^* \right]. \quad (13)$$

The parameters are given as follows:

$$A(t_f, t_i) = -\frac{1}{V} e^2 l^2(\omega) \int_{t_i}^{t_f} d\tau \int_{t_i}^{\tau} d\rho \mathcal{G}(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i\vec{k}_{ph} \cdot \vec{r}(\tau)} \mathcal{G}(\rho) \hat{\varepsilon}^* \cdot \vec{r}(\rho) e^{-i\vec{k}_{ph} \cdot \vec{r}(\rho)} e^{-i\omega(\tau-\rho)}, \quad (14)$$

$$B(t_f - t_i) = 1 - Y(t_f, t_i) = 1 - e^{-i\omega(t_f-t_i)}, \quad (15)$$

$$D(t_f, t_i) = \frac{1}{\sqrt{V}} e l(\omega) \int_{t_i}^{t_f} d\tau \mathcal{G}(\tau) \hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i\vec{k}_{ph} \cdot \vec{r}(\tau)} e^{-i\omega(t_f-\tau)}, \quad (16)$$

$$D_1(t_f, t_i) = -\frac{1}{\sqrt{V}} e l(\omega) \int_{t_i}^{t_f} d\tau \mathcal{G}(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i\vec{k}_{ph} \cdot \vec{r}(\tau)} e^{-i\omega(\tau-t_i)}. \quad (17)$$

In the case of a field transition between an initial photonic state $|\Phi_1\rangle$ and a final one $|\Phi_2\rangle$, the reduced propagator of finite time takes the form

$$\tilde{K}(\vec{r}_f, t_f; \vec{r}_i, t_i) = \int \frac{d^2\alpha}{\pi} e^{|\alpha|^2} \langle \Phi_2 | \alpha \rangle K(\alpha, \vec{r}_f, t_f; \alpha, \vec{r}_i, t_i) \langle \alpha | \Phi_1 \rangle. \quad (18)$$

Here we consider that we have a field transition from an initial coherent state $|\beta\rangle$ to a final one $|\gamma\rangle$. So we can integrate to obtain the following reduced propagator for the motion of the electron,

$$\tilde{K}(\vec{r}_f, t_f; \vec{r}_i, t_i) = C(t_f - t_i) K_0(\vec{r}_f, t_f; \vec{r}_i, t_i) \\ = C(t_f - t_i) \int \int D\vec{r}(\tau) \frac{D\vec{p}(\tau)}{(2\pi)^3} \exp \{ i S_{\text{tot}}[\vec{p}, \vec{r}, \tau] \}, \quad (19)$$

where

$$C(t) = \frac{\exp\left(\frac{\beta\gamma^*}{B(t)} - \frac{1}{2}|\beta|^2 - \frac{1}{2}|\gamma|^2\right)}{B(t)}. \quad (20)$$

The action is

$$\begin{aligned} S_{\text{tot}}[\vec{p}, \vec{r}, \tau] = & \int_{t_i}^{t_f} \left[\vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau)) \right] d\tau \\ & + i \frac{1}{\sqrt{V}} e l(\omega) \int_{t_i}^{t_f} d\tau \left(\beta \chi(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i \vec{k}_{ph} \cdot \vec{r}(\tau)} + \gamma^* \chi^*(\tau) \hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i \vec{k}_{ph} \cdot \vec{r}(\tau)} \right) \\ & + \frac{1}{V} e^2 l^2(\omega) \int_{t_i}^{t_f} d\tau \wp(\tau) \int_{t_i}^{\tau} d\rho \wp(\rho) \left[i \frac{e^{i\omega(\tau-\rho)}}{e^{i\omega(t_f-t_i)} - 1} \left(\hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i \vec{k}_{ph} \cdot \vec{r}(\tau)} \right) \left(\hat{\varepsilon} \cdot \vec{r}(\rho) e^{i \vec{k}_{ph} \cdot \vec{r}(\rho)} \right) + c.c. \right], \end{aligned} \quad (21)$$

where $\chi(\tau)$ has the form

$$\chi(\tau) = \wp(\tau) \frac{e^{-i\omega\tau}}{e^{-i\omega t_i} - e^{-i\omega t_f}}. \quad (22)$$

We notice the following identities:

$$\frac{1}{B(t)} = \frac{1}{2} - \frac{1}{2} i \cot\left(\frac{\omega t}{2}\right) = \frac{1}{2} - \frac{i}{\omega} \sum_{m=-\infty}^{\infty} \frac{1}{t - \frac{2\pi m}{\omega}}. \quad (23)$$

On using them and for arbitrary $A(t)$ we can obtain the following formula after a direct Fourier transform,

$$\int_{-\infty}^{\infty} \frac{A(t)}{B(t)} e^{ift} dt = \frac{1}{2} \int_{-\infty}^{\infty} A(t) e^{ift} dt + \frac{\pi}{\omega} \sum_{m=-\infty}^{\infty} A\left(\frac{2\pi m}{\omega}\right) \exp\left(if \frac{2\pi m}{\omega} \right). \quad (24)$$

Finally, upon using an inverse Fourier transform we obtain the following functional identities

$$\frac{A(t)}{B(t)} = A(t) \left[\frac{1}{2} + \frac{\pi}{\omega} \sum_{m=-\infty}^{\infty} \delta\left(\frac{2\pi m}{\omega} - t\right) \right] = A(t) \left[\frac{1}{2} + \frac{1}{2} \sum_{m=-\infty}^{\infty} \delta\left(m - \frac{\omega t}{2\pi}\right) \right]. \quad (25)$$

In the above expressions, the summation is to be performed symmetrically. Identity in Eq. (25) is to be used in Eqs. (19) and (20). The delta functions do not contribute in the final expressions of Section 4 at the specific times introduced by them the photonic influence functional becomes zero. Moreover, the measure of all those times is zero. Further to handle the exponential in Eq. (20) within the scattering theory of Section 4 we use the limit

$$\lim_{t \rightarrow \infty} \frac{1}{B(t)} = \lim_{t \rightarrow \infty} \frac{1}{1 - \exp(-i(\omega - i0)t)} = 1. \quad (26)$$

Now due to the large volume V , we shall approximate the exact action (21) by neglecting in the Taylor expansions

$$\vec{r}(\rho) = \vec{r}(\tau) + (\rho - \tau)\dot{\vec{r}}(\tau) + \dots, \quad (27)$$

higher terms than the first one, as they are going to involve powers of higher order in V in the denominator. To demonstrate this we consider the action in Eq. (21) and we derive the equation of motion of the electron by using Lagrange's equation and the action's Lagrangian in the absence of $V(\vec{r})$. So the part of the Lagrangian that interests us reads

$$\begin{aligned} L = & \frac{\dot{\vec{r}}^2(\tau)}{2} + \frac{1}{\sqrt{V}} el(\omega) \left(\beta\chi(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i\vec{k}_{ph} \cdot \vec{r}(\tau)} + \gamma^* \chi^*(\tau) \hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i\vec{k}_{ph} \cdot \vec{r}(\tau)} \right) \\ & + \frac{1}{V} e^2 l^2(\omega) \mathcal{G}(\tau) \int_{t_i}^{\tau} d\rho \mathcal{G}(\rho) \left[i \frac{e^{i\omega(\tau-\rho)}}{e^{i\omega(t_f-t_i)} - 1} \left(\hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i\vec{k}_{ph} \cdot \vec{r}(\tau)} \right) \left(\hat{\varepsilon} \cdot \vec{r}(\rho) e^{i\vec{k}_{ph} \cdot \vec{r}(\rho)} \right) + c.c. \right], \end{aligned} \quad (28)$$

and has equation of motion

$$\ddot{\vec{r}}(\tau) = O\left(\frac{1}{\sqrt{V}}\right). \quad (29)$$

Therefore we can set,

$$\vec{r}(\rho) = \vec{r}(\tau) + O\left(\frac{1}{\sqrt{V}}\right). \quad (30)$$

In the case of the presence of $V(\vec{r})$ we perform a full order perturbation expansion of the full propagator in Eq. (19) with respect to the potential term. That is,

$$K_0 = T + TVT + TVTVT + \dots \quad (31)$$

Then the propagator T , in the expansion, will be the one of the electron in the photonic field for which the approximation of Eq. (30) as discussed above is valid. Then, we sum back to obtain the final full propagator, thus maintaining the same approximation for the total propagator as well. Notice that the expansion (31) may converge very slowly but since it is a full order expansion it does not matter. Eventually in the large volume limit we get the action

$$S_{\text{tot}}[\vec{p}, \vec{r}, \tau] = \int_{t_i}^{t_f} \left[\vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau)) \right] d\tau \\
+ i \frac{1}{\sqrt{V}} e l(\omega) \int_{t_i}^{t_f} d\tau \left(\beta \chi(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) e^{i \vec{k}_{\text{ph}} \cdot \vec{r}(\tau)} + \gamma^* \chi^*(\tau) \hat{\varepsilon}^* \cdot \vec{r}(\tau) e^{-i \vec{k}_{\text{ph}} \cdot \vec{r}(\tau)} \right) \quad (32) \\
+ \frac{1}{V} e^2 l^2(\omega) \int_{t_i}^{t_f} d\tau v(\tau) \left| \hat{\varepsilon} \cdot \vec{r}(\tau) \right|^2,$$

where

$$v(\tau) = \wp(\tau) \int_{t_i}^{\tau} \wp(\rho) \xi(\tau - \rho) d\rho, \quad (33)$$

$$\xi(\tau - \rho) = \csc \left[\frac{\omega(t_f - t_i)}{2} \right] \cos \left[\omega(\tau - \rho) - \frac{\omega(t_f - t_i)}{2} \right]. \quad (34)$$

Finally, we notice that in the long wavelength approximation we can set $e^{i \vec{k}_{\text{ph}} \cdot \vec{r}} \cong 1$. So we obtain the following expression

$$S_{\text{tot}}[\vec{p}, \vec{r}, \tau] = \int_{t_i}^{t_f} \left[\vec{p}(\tau) \cdot \dot{\vec{r}}(\tau) - \frac{\vec{p}^2(\tau)}{2} - V(\vec{r}(\tau)) \right] d\tau + \\
i \frac{1}{\sqrt{V}} e l(\omega) \int_{t_i}^{t_f} d\tau \left[\beta \chi(\tau) \hat{\varepsilon} \cdot \vec{r}(\tau) + \gamma^* \chi^*(\tau) \hat{\varepsilon}^* \cdot \vec{r}(\tau) \right] + \quad (35) \\
\frac{1}{V} e^2 l^2(\omega) \int_{t_i}^{t_f} d\tau v(\tau) \left| \hat{\varepsilon} \cdot \vec{r}(\tau) \right|^2.$$

Now we proceed to the angular decomposition of the above expressions.

3. Angular decomposition

We intend to perform angular decomposition and evaluate the SSP corresponding to the propagator of Eq. (19) in the long wavelength approximation.

Here we consider elliptic polarization so that the polarization vector takes the form

$$\hat{\varepsilon} = \hat{\varepsilon}_x \cos \left(\frac{\xi}{2} \right) \pm i \hat{\varepsilon}_y \sin \left(\frac{\xi}{2} \right), \quad (36)$$

where $\widehat{\varepsilon}_x$ and $\widehat{\varepsilon}_y$ are the unit vectors along the x - and y -axis. The upper sign corresponds to left polarization while the lower one to right one.

The propagator $K_0^\xi(\vec{r}_f, t_f; \vec{r}_i, t_i)$ of Eq. (19) with the above polarization vector $\widehat{\varepsilon}$ has the discrete form

$$K_0^\xi(\vec{r}_f, t_f; \vec{r}_i, t_i) = \prod_{n=1}^N \left[\int_{-\infty}^{\infty} d\vec{r}_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_n}{(2\pi)^3} \right] \times \exp \left\{ i \sum_{n=1}^{N+1} \left[\vec{p}_n \cdot (\vec{r}_n - \vec{r}_{n-1}) - \varepsilon \left(\frac{\vec{p}_n^2(\tau)}{2} + V(\vec{r}_n) \right) \right. \right. \\ \left. \left. + i \sqrt{\frac{2\pi\omega}{V}} \varepsilon (\beta \chi_n \widehat{\varepsilon} \cdot \vec{r}_n + \gamma^* \chi_n^* \widehat{\varepsilon}^* \cdot \vec{r}_n) + \frac{2\pi\omega}{V} \varepsilon v_n \left| \widehat{\varepsilon} \cdot \vec{r}_n \right|^2 \right] \right\}. \quad (37)$$

All the functions with index n are evaluated at time $\tau_n = n\varepsilon + t_i$ where $\varepsilon = \frac{t_f - t_i}{N+1}$. χ_n and v_n have the form (see Eqs. (22) and (33))

$$\chi_n = \wp(\tau_n) \frac{e^{-i\omega\tau_n}}{e^{-i\omega t_i} - e^{-i\omega t_f}}, \quad (38)$$

$$v_n = v(\tau_n). \quad (39)$$

Additionally, we note that we have set $\vec{r}_0 = \vec{r}_i$ and $\vec{r}_{N+1} = \vec{r}_f$.

Now we insert delta functions in Eq. (37) to get the expression

$$K_0^\xi(\vec{r}_f, t_f; \vec{r}_i, t_i) = \prod_{n=1}^N \left[\int_{-\infty}^{\infty} d\vec{r}_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} \frac{d\vec{p}_n}{(2\pi)^3} \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^{\infty} d^2 w_n \right] \prod_{n=1}^{N+1} [\delta^{(2)}(w_n - \widehat{\varepsilon} \cdot \vec{r}_n)] \\ \times \exp \left\{ i \sum_{n=1}^{N+1} \left[\vec{p}_n \cdot (\vec{r}_n - \vec{r}_{n-1}) - \varepsilon \left(\frac{\vec{p}_n^2(\tau)}{2} + V(\vec{r}_n) \right) \right. \right. \\ \left. \left. + i \sqrt{\frac{2\pi\omega}{V}} \varepsilon (\beta \chi_n w_n + \gamma^* \chi_n^* w_n^*) + \frac{2\pi\omega}{V} \varepsilon v_n \left| w_n \right|^2 \right] \right\}. \quad (40)$$

We have defined $\delta^{(2)}(z) = \delta(z)\delta(z^*)$. Moreover $w_n = w_{xn} + iw_{yn}$. The delta functions have the representation

$$\begin{aligned} \delta^{(2)}(w_n - \hat{\varepsilon} \cdot \vec{r}_n) = & \delta^{(2)}\left(w_n - r_n \left[\sin \vartheta_n \left(\cos \left(\frac{\xi}{2} \right) \cos \varphi_n \pm i \sin \left(\frac{\xi}{2} \right) \sin \varphi_n \right) \right]\right) = \frac{1}{(2\pi)^2} \\ & \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d^2 \lambda_n \exp \left[i \frac{1}{2} (\lambda_n w_n + \lambda_n^* w_n^*) - i \frac{1}{2} \lambda_n \left(\hat{\varepsilon}_x \cos \left(\frac{\xi}{2} \right) \pm i \hat{\varepsilon}_y \sin \left(\frac{\xi}{2} \right) \right) \cdot \vec{r}_n \right. \\ & \left. - i \frac{1}{2} \lambda_n^* \left(\hat{\varepsilon}_x \cos \left(\frac{\xi}{2} \right) \mp i \hat{\varepsilon}_y \sin \left(\frac{\xi}{2} \right) \right) \cdot \vec{r}_n \right] = \frac{1}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d^2 \lambda_n \\ & \times \exp \left[i \lambda_{xn} w_{xn} - i \lambda_{yn} w_{yn} - i \lambda_{xn} \cos \left(\frac{\xi}{2} \right) \hat{\varepsilon}_x \cdot \vec{r}_n \pm i \lambda_{yn} \sin \left(\frac{\xi}{2} \right) \hat{\varepsilon}_y \cdot \vec{r}_n \right]. \end{aligned} \quad (41)$$

We have set $\lambda_n = \lambda_{xn} + i \lambda_{yn}$. Now we perform the change of variables $\lambda_{xn} \rightarrow \frac{\lambda_{xn}}{\cos(\frac{\xi}{2})}$, $\lambda_{yn} \rightarrow \frac{\lambda_{yn}}{\sin(\frac{\xi}{2})}$, $w_{xn} \rightarrow \cos(\frac{\xi}{2}) w_{xn}$, $w_{yn} \rightarrow \sin(\frac{\xi}{2}) w_{yn}$. The factor due to the integration on λ_n is cancelled with the factor due to the integration on w_n . Further we expand angularly according to the identity,

$$e^{i \vec{k} \cdot \vec{r}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^l i^l j_l(|\vec{k}|r) Y_{lm}^*(\vartheta_k, \varphi_k) Y_{lm}(\vartheta, \varphi), \quad (42)$$

where j_l are spherical Bessel functions, and Y_{lm} are spherical harmonics. So for right elliptic polarization we get

$$\delta^{(2)}(w_n - \hat{\varepsilon} \cdot \vec{r}_n) = \sum_{l_n=0}^{\infty} \sum_{m_n=-l_n}^{l_n} g_{l_n m_n}(w'_n, r_n) \sqrt{4\pi} Y_{l_n m_n}(\vartheta_n, \varphi_n), \quad (43)$$

where

$$g_{l_n m_n}(w'_n, r_n) = (-i)^{l_n} \frac{O_{l_n m_n}}{(2\pi)^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d^2 \lambda_n \exp [i \lambda_{xn} w'_{xn} - i \lambda_{yn} w'_{yn}] \quad (44)$$

$$\times j_{l_n}(|\lambda_n| r_n) \exp(-i m_n \varphi_{\lambda_n}),$$

$$\begin{aligned} O_{l_n m_n} &= \sqrt{(2l_n + 1) \frac{(l_n - m_n)!}{(l_n + m_n)!}} P_{l_n}^{m_n}(0) \\ &= \sqrt{(2l_n + 1) \frac{(l_n - m_n)!}{(l_n + m_n)!}} \frac{\sqrt{\pi} 2^{m_n}}{\Gamma\left(\frac{l_n - m_n}{2} + 1\right) \Gamma\left(\frac{-l_n - m_n + 1}{2}\right)}. \end{aligned} \quad (45)$$

We notice that if $l_n + m_n$ is odd then $O_{l_n m_n}$ is zero. Moreover $|\lambda_n|$, φ_{λ_n} are the polar coordinates of λ_n on the x - y plane. We have set

$$w_{xn} = w'_{xn} \cos\left(\frac{\xi}{2}\right) = |w'_n| \cos(\varphi_{w'_n}) \cos\left(\frac{\xi}{2}\right), \quad (46)$$

$$w_{yn} = w'_{yn} \sin\left(\frac{\xi}{2}\right) = |w'_n| \sin(\varphi_{w'_n}) \sin\left(\frac{\xi}{2}\right), \quad (47)$$

and

$$w'_n = w'_{xn} + iw'_{yn} = |w'_n| e^{i\varphi_{w'_n}}. \quad (48)$$

On integrating over φ_{λ_n} we get

$$\begin{aligned} g_{l_n m_n}(w'_n, r_n) &= (-i)^{l_n} \frac{O_{l_n m_n}}{2\pi} \exp\left(im_n\left(\varphi_{w'_n} + \frac{\pi}{2}\right)\right) \\ &\times \int_0^\infty d\rho_{\lambda_n} \rho_{\lambda_n} j_{l_n}(\rho_{\lambda_n} r_n) J_{m_n}(\rho_{\lambda_n} |w'_n|). \end{aligned} \quad (49)$$

$\rho_{\lambda_n} = |\lambda_n|$ and J_{m_n} are Bessel functions. In the appendix we give results for the expression in Eq. (49).

Finally, we replace the delta functions in Eq. (40) with the above angularly decomposed expressions. As $N \rightarrow \infty$ and within the range from $n = 0$ to N we keep first-order angular terms. Higher order angular parts would contribute infinities. Finally, the propagator takes the form

$$\begin{aligned} K_0^\xi(\vec{r}_f, t_f; \vec{r}_i, t_i) &= \\ &\frac{1}{r_f r_i} \sum_{l=0}^\infty \sum_{m=-l}^l \sum_{q=0}^\infty \sum_{p=-q}^q K_{lmq}^\xi(r_f, t_f; r_i, t_i) \sqrt{4\pi} Y_{lm}(\vartheta_f, \varphi_f) Y_{qp}(\vartheta_f, \varphi_f) Y_{qp}^*(\vartheta_i, \varphi_i), \end{aligned} \quad (50)$$

where after standard manipulations [11] on the angular parts of the atomic system $K_{lmq}^\xi(r_f, t_f; r_i, t_i)$ takes the form

$$\begin{aligned} K_{lmq}^\xi(r_f, t_f; r_i, t_i) &= \prod_{n=1}^N \left[\int_0^\infty dr_n \right] \prod_{n=1}^{N+1} \left[\int_{-\infty}^\infty \frac{dp_n}{2\pi} \right] \prod_{n=1}^{N+1} \left[\iint_{|w'_n| < r_n} d^2 w'_n \right] \prod_{n=1}^N [g_{00}(w'_n, r_n)] \\ &\times g_{lm}(w'_{N+1}, r_{N+1}) \exp \left\{ i \sum_{n=1}^{N+1} \left[p_n(r_n - r_{n-1}) - \varepsilon \left(\frac{p_n^2}{2} + \frac{q(q+1)}{2r_n^2} + V(r_n) \right) \right. \right. \\ &\left. \left. + i \sqrt{\frac{2\pi\omega}{V}} \varepsilon (\beta \chi_n w_n + \gamma^* \chi_n^* w_n^*) + \frac{2\pi\omega}{V} \varepsilon v_n |w_n|^2 \right] \right\}. \end{aligned} \quad (51)$$

Further we observe that

$$\begin{aligned} & \lim_{N \rightarrow \infty} \prod_{n=1}^N \left[\iint_{|w'_n| < r_n} d^2 w'_n \right] \prod_{n=1}^N [g_{00}(w'_n, r_n)] \\ & \times \exp \left\{ i \frac{t_f - t_i}{N+1} \sum_{n=1}^N \left[i \sqrt{\frac{2\pi\omega}{V}} (\beta \chi_n w_n + \gamma^* \chi_n^* w_n^*) + \frac{2\pi\omega}{V} v_n |w_n|^2 \right] \right\} \\ & = \exp \left\{ i \frac{2\pi\omega}{3V} \int_{t_i}^{t_f} d\tau [\nu(\tau) r^2(\tau)] \right\}. \end{aligned} \quad (52)$$

So Eq. (51) becomes

$$\begin{aligned} K_{\text{lmq}}^\xi(r_f, t_f; r_i, t_i) &= F_{\text{lm}}(r_f) \iint Dr(\tau) \frac{Dp(\tau)}{2\pi} \\ &\times \exp \left\{ i \int_{t_i}^{t_f} d\tau \left[p\dot{r} - \left(\frac{p^2}{2} + \frac{q(q+1)}{2r^2} + V(r) \right) \right] + i \frac{2\pi\omega}{3V} \int_{t_i}^{t_f} \nu(\tau) r^2(\tau) d\tau \right\}, \end{aligned} \quad (53)$$

where

$$\begin{aligned} F_{\text{lm}}(r_f) &= \iint_{|w'_f| < r_f} d^2 w'_f g_{\text{lm}}(w'_f, r_f) \times \\ &\exp \left\{ -\sqrt{\frac{2\pi\omega}{V}} \varepsilon (\beta \chi w_f + \gamma^* \chi^* w_f^*) + i \frac{2\pi\omega}{V} \varepsilon v |w_f|^2 \right\}. \end{aligned} \quad (54)$$

We notice that to evaluate the integrals in Eq. (54) we have to take into account the expressions of Eqs. (46) and (47). Then we expand it on parameters of interest and integrate on time.

In the next section, we use the present propagator in its SSP form which appears after the solution of the sign problem. It is

$$\begin{aligned} K_1^\xi(\vec{r}_f, t; \vec{r}_i, 0) &= \frac{1}{r_f r_i} \delta(r_f - r_i) \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{q=0}^{\infty} \sum_{p=-q}^q Y_{\text{qp}}(\vartheta_f, \varphi_f) Y_{\text{qp}}^*(\vartheta_i, \varphi_i) \\ &\times \sqrt{4\pi} Y_{\text{lm}}(\vartheta_f, \varphi_f) F_{\text{lm}}(r_f) \exp \left[i \frac{2\pi\omega}{3V} r_f^2 \int_0^t \nu(\tau) d\tau \right]. \end{aligned} \quad (55)$$

We have dropped the phase due to the atomic Hamiltonian because in the subsequent application of the present chapter, it eventually cancels.

4. Application and results

Proceeding to an application of the present theory we apply the above formalism to the case of the ionization of hydrogen. In that case the potential is given as

$$V(\vec{r}) = -\frac{1}{r}. \quad (56)$$

We use as an initial state, the hydrogen's ground one with wavefunction,

$$\Psi_i(\vec{r}, t) = \Psi_i(\vec{r})e^{-i\varepsilon_i t} = R_{1s}(r)Y_{00}(\vartheta, \phi)e^{-i\varepsilon_i t} = 2e^{-r}Y_{00}(\vartheta, \phi)e^{-i\varepsilon_i t}, \quad (57)$$

where $\varepsilon_i = -1/2$ is the energy of the ground $H(1s)$ state.

The final state of the ionized electron with wave vector $\vec{k} = k(\sin \vartheta_k \cos \varphi_k, \sin \vartheta_k \sin \varphi_k, \cos \vartheta_k)$ is

$$\begin{aligned} \Psi_f^{\vec{k}}(\vec{r}, t) = \\ \Psi_f^{\vec{k}}(\vec{r})e^{-i\varepsilon t} = \exp\left(\frac{\pi}{2k}\right)\Gamma\left(1 + \frac{i}{k}\right)e^{i\vec{k} \cdot \vec{r}} {}_1F_1\left(-\frac{i}{k}; 1; -ikr - i\vec{k} \cdot \vec{r}\right)e^{-i\varepsilon t}. \end{aligned} \quad (58)$$

It has energy

$$\varepsilon = k^2/2, \quad (59)$$

and partial wave expansion

$$\Psi_f^{\vec{k}}(\vec{r}) = \frac{2\pi}{k} \sum_{s=0}^{\infty} i^s e^{-i\delta_s} R_s^k(r) \sum_{t=-s}^s Y_{st}^*(\vartheta, \phi) Y_{st}(\vartheta_k, \phi_k). \quad (60)$$

$$\begin{aligned} R_s^k(r) = \frac{\sqrt{8\pi k}}{\sqrt{1 - \exp(-2\pi/k)}} \prod_{y=1}^s \left(\sqrt{y^2 + \frac{1}{k^2}} \right) \frac{1}{(2s+1)!} \\ \times (2kr)^s e^{-ikr} {}_1F_1\left(\frac{i}{k} + s + 1, 2s + 2, 2ikr\right) \end{aligned} \quad (61)$$

is the radial function and $\delta_s = \arg \Gamma(1 - \frac{i}{k} + s)$ a phase. Then the transition amplitude from the initial state i at $t \rightarrow -\infty$ to the final continuum state f at $t \rightarrow +\infty$ may be evaluated at any time t ; it is

$$A_{fi} = \langle \Phi_f^-(t) | \Phi_i^+(t) \rangle, \quad (62)$$

where $\Phi_f^-(\vec{r}, t)$ and $\Phi_i^+(\vec{r}, t)$ are exact solutions of the present system's time-dependent Schrodinger equation subject to the asymptotic conditions

$$\Phi_f^-(\vec{r}, t) \xrightarrow{t \rightarrow +\infty} \Psi_f^k(\vec{r}, t), \quad (63)$$

$$\Phi_i^+(\vec{r}, t) \xrightarrow{t \rightarrow -\infty} \Psi_i(\vec{r}, t). \quad (64)$$

According to standard scattering theory we obtain the following form of the transition amplitude

$$A_{fi} = \frac{1}{2} \lim_{\substack{t_1 \rightarrow -\infty \\ t_2 \rightarrow \infty}} \left\langle \Psi_f^k \left| U^0(t_2)^+ \exp \left(-i \int_0^{t_2} H_{eff}(t_2, \rho) d\rho + i \int_0^{t_1} H_{eff}(t_1, \rho) d\rho \right) U^0(t_1) \right| \Psi_i \right\rangle. \quad (65)$$

The effective Hamiltonian H_{eff} , appearing above and corresponding to the action of Eq. (35) has the form (see Eq. (2))

$$H_{eff} = H_e - i \frac{1}{\sqrt{V}} el(\omega) (\beta \chi \hat{\varepsilon} \cdot \vec{r} + \beta^* \chi^* \hat{\varepsilon}^* \cdot \vec{r}) - \frac{1}{V} e^2 l^2(\omega) v |\hat{\varepsilon} \cdot \vec{r}|^2. \quad (66)$$

Moreover

$$U^0(t) = e^{-iH_e t}. \quad (67)$$

We set $\beta = \gamma$. This appears to be a requirement in order the Hamiltonian to be PT (parity–time reversal) symmetric. The one-half factor in Eq. (65) appears due to the initial $\frac{1}{B(t)}$ factor in Eq. (20) and the identity in Eq. (25). At the times introduced by the delta functions the propagator $K_1^\xi(\vec{r}_f, \tau; \vec{r}_i, 0)$ (see below) becomes zero. Moreover the exponential in Eq. (20) is one as $\lim_{t \rightarrow \infty} \frac{1}{B(t)} = 1$ and $\beta = \gamma$.

Now to proceed we set $t_2 = -t_1 = t$ and take into account the PT invariance of the whole system as the Hamiltonian Eq. (66) is PT invariant. So we reverse the time sign of the terms involving the time t_1 something that equivalently implies for the position $\vec{r} \rightarrow -\vec{r}$, for the momentum $\vec{p} \rightarrow \vec{p}$ and for the imaginary unit $i \rightarrow -i$. Then we differentiate the operators between the bra and the ket in Eq. (65), with respect to the variable t . Finally, after certain standard manipulations and a subsequent integration we obtain the result

$$\begin{aligned} A_{fi} = & \left\langle \Psi_f^k \left| \Psi_i \right. \right\rangle + \\ & + \int_0^\xi d\tau \left\langle \Psi_f^k \left| U^0(\tau)^+ \exp \left(-i \int_0^\tau H_{eff}(\tau, \rho) d\rho + i \int_{-\tau}^0 H_e(\rho) d\rho \right) \right. \right. \\ & \times \left(-\frac{1}{\sqrt{V}} el(\omega) (\beta \chi \hat{\varepsilon} \cdot \vec{r} + \beta^* \chi^* \hat{\varepsilon}^* \cdot \vec{r}) + i \frac{1}{V} e^2 l^2(\omega) v |\hat{\varepsilon} \cdot \vec{r}|^2 \right) U^0(\tau) \left. \right| \Psi_i \right\rangle. \end{aligned} \quad (68)$$

We have supposed that the duration of the pulse is ζ , as well as that it begins at time zero. Now in order to proceed we take into account that the asymptotic initial and final states are orthogonal. Further we make use of the path-integral representation of the exponential in Eq. (68) and angularly decompose it. So on making use of the results of the previous section and solving the sign problem [8], Eq. (68) becomes

$$A_{fi} = \int_0^\zeta d\tau \iint d\vec{r}_f d\vec{r}_i \frac{1}{r_i^2} e^{i(\varepsilon - \varepsilon_i)\tau} \left(\Psi_f^{\vec{k}}(\vec{r}_f) \right)^* K_1^\xi(\vec{r}_f, \tau; \vec{r}_i, 0) \times \left(-\sqrt{\frac{2\pi\omega}{V}} (\beta\chi(\tau)\hat{\varepsilon} \cdot \vec{r}_i + c.c.) + i\frac{2\pi\omega}{V} |\hat{\varepsilon} \cdot \vec{r}_i|^2 \nu(\tau) \right) \Psi_i(\vec{r}_i). \quad (69)$$

We have used the prior form of the transition amplitude. $K_1^\xi(\vec{r}_f, \tau; \vec{r}_i, 0)$ is given by Eq. (55). The phase which appears after the solution of the sign problem has cancelled.

As the present theory is PT symmetric we have to use PT symmetric quantum mechanics. So our equations take their final form according to the fact that $\left(\Psi_f^{\vec{k}}(\vec{r}) \right)^{PT} = \left(\Psi_f^{\vec{k}}(\vec{r}) \right)^*$.

Here we want to study two-photon ionization processes. They are of order $\frac{1}{V}$ or higher. For the same transitions the vacuum fluctuations term contributes to the same order. So we take it into account. The amplitude takes the form

$$A = \int_0^\zeta d\tau \iint d\vec{r}_f d\vec{r}_i \frac{1}{r_i^2} e^{i(\varepsilon - \varepsilon_i)\tau} \left(\Psi_f^{\vec{k}}(\vec{r}_f) \right)^* \times \left(-\sqrt{\frac{2\pi\omega}{V}} S_{l=1}^\xi(\vec{r}_f, \tau; \vec{r}_i, 0) (\beta\chi(\tau)\hat{\varepsilon} \cdot \vec{r}_i + c.c.) + i\frac{2\pi\omega}{V} S_{l=0}^\xi(\vec{r}_f, \tau; \vec{r}_i, 0) |\hat{\varepsilon} \cdot \vec{r}_i|^2 \nu(\tau) \right) \Psi_i(\vec{r}_i). \quad (70)$$

Upon expanding to powers of volume the sign solved propagators appearing in Eq. (70) take the form

$$S_{l=1}^\xi(\vec{r}_f, \tau; \vec{r}_i, 0) = \frac{1}{r_f r_i} \delta(r_f - r_i) \sum_{q=0}^\infty \sum_{p=-q}^q Y_{qp}(\vartheta_f, \varphi_f) Y_{qp}^*(\vartheta_i, \varphi_i) \times \left[-\sqrt{\frac{2\pi\omega}{V}} (\hat{\varepsilon} \cdot \vec{r}_f \beta \int_0^\tau d\rho \chi(\rho) + c.c.) \right] \exp \left[i\frac{2\pi\omega}{3V} r_f^2 \int_0^\tau \nu(\rho) d\rho \right], \quad (71)$$

and

$$S_{l=0}^{\xi}(\vec{r}_f, \tau; \vec{r}_i, 0) = \frac{1}{r_f r_i} \delta(r_f - r_i) \sum_{q=0}^{\infty} \sum_{p=-q}^q Y_{qp}(\vartheta_f, \varphi_f) Y_{qp}^*(\vartheta_i, \varphi_i) \times \left\{ 1 + \frac{2\pi\omega}{3V} r_f^2 \left(i \int_0^{\tau} v(\rho) d\rho + \left| \beta \int_0^{\tau} d\rho \chi(\rho) \right|^2 + \cos \xi \operatorname{Re} \left[\left(\beta \int_0^{\tau} d\rho \chi(\rho) \right)^2 \right] \right) \right\} \times \exp \left[i \frac{2\pi\omega}{3V} r_f^2 \int_0^{\tau} v(\rho) d\rho \right]. \quad (72)$$

Finally, we obtain the second-order transition probability

$$\frac{\partial P}{\partial \varepsilon} = \frac{1}{4\pi^2} k \int |A|^2 d\Omega_{\vec{k}}. \quad (73)$$

Here we consider the case of an orthogonal pulse of duration ζ . Then

$$\wp(\tau) = \begin{cases} 1 & 0 \leq \tau \leq \zeta \\ 0 & \text{otherwise} \end{cases}. \quad (74)$$

In **Figure 1**, we plot the second-order term $\frac{\partial P}{\partial \varepsilon}$ as a function of the energy of the injected electron ε for $\zeta = 100$ as and various values of the elliptic polarization parameter ξ . We use

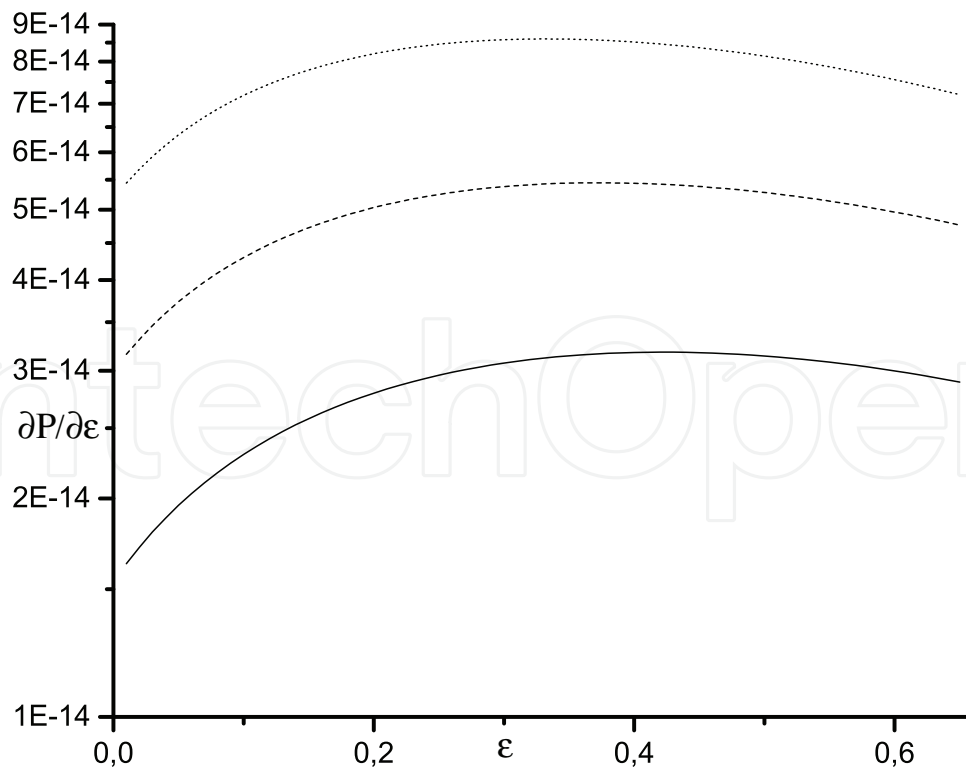


Figure 1. Second-order probability $\frac{\partial P}{\partial \varepsilon}$ of ionization as a function of the ε . We set $\zeta = 100$ as. We give curves corresponding to $\xi = \frac{\pi}{2}$ (solid) $\xi = \frac{\pi}{3}$ (dashed) $\xi = \frac{\pi}{20}$ (dotted). We use $\omega = 0.4275$ a.u., $\beta = 1$ and $V = 10^7$.

$2\omega = 0.855$ a.u. Within the range $0 \leq \xi \leq \frac{\pi}{2}$ the larger the ξ the smaller the transition probability. $\xi = \frac{\pi}{2}$ corresponds to circular polarization. We give another approach of this case in [10]. $\xi = 0$ corresponds to linear polarization. In that case the present approach is degenerate. We give other approaches in [6, 7, 9].

5. Conclusions

In the present chapter we have used path-integral methods in the study of the interaction of electrons with photonic states. We have integrated the photonic field and then angularly decomposed the electron–photonic field influence functional. Within those manipulations there have appeared terms due to the electromagnetic vacuum fluctuations.

As an application we have developed a scattering theory and used it in the two-photon ionization of hydrogen. For those transitions, the electromagnetic vacuum fluctuations contribute to the same order. Moreover to handle the path integrals that appear, we have used the relevant propagators in their sign solved propagator (SSP) form. The SSP theory appears in Ref. [8].

Concluding the present method is tractable and can be used in many problems involving the quantum mechanics of one-electron atoms interacting with radiation.

Appendix

In Eq. (49), we have the expression (here we drop the n indices)

$$\begin{aligned}
 g_{lm}(w', r) &= (-i)^l \frac{O_{lm}}{2\pi} \exp\left(im\left(\varphi_{w'} + \frac{\pi}{2}\right)\right) \int_0^\infty d\rho_\lambda \rho_\lambda j_l(\rho_\lambda r) J_m(\rho_\lambda |w'|) \\
 &= \frac{O_{lm}}{2\pi} (-i)^l i^m e^{im\varphi_{w'}} \sqrt{\frac{\pi}{2r}} \int_0^\infty d\rho_\lambda \sqrt{\rho_\lambda} J_{l+\frac{1}{2}}(\rho_\lambda r) J_m(\rho_\lambda |w'|) \\
 &= \frac{O_{lm}}{2\pi} i^m (-i)^l e^{im\varphi_{w'}} \frac{\sqrt{\pi} |w'|^m \Gamma\left(\frac{l+m}{2} + 1\right)}{r^{m+2} \Gamma\left(\frac{l-m+1}{2}\right) \Gamma(m+1)} \\
 &\quad \times F\left(\frac{l+m}{2} + 1, \frac{m-l+1}{2}; m+1; \frac{|w'|^2}{r^2}\right) \Theta(r - |w'|) \\
 &= \frac{O_{lm}}{2\pi} i^m (-i)^l e^{im\varphi_{w'}} \frac{2^m \sqrt{\pi} \Gamma\left(\frac{l+m}{2} + 1\right)}{r \Gamma\left(\frac{l-m+1}{2}\right)} \frac{1}{\sqrt{r^2 - |w'|^2}} \\
 &\quad \times P_l^{-m}\left(\frac{\sqrt{r^2 - |w'|^2}}{r}\right) \Theta(r - |w'|),
 \end{aligned} \tag{75}$$

where $\Theta(x)$ is the step function

$$\Theta(x) = \begin{cases} 1, & x > 0 \\ 0, & x < 0 \end{cases}. \quad (76)$$

We give the following cases:

$$g_{00}(w', r) = \frac{1}{2\pi} \frac{1}{r\sqrt{r^2 - |w'|^2}} \Theta(r - |w'|), \quad (77)$$

$$g_{1\pm 1}(w', r) = \mp \sqrt{\frac{3}{2}} \frac{e^{\pm i\varphi_{w'}}}{2\pi} \frac{|w'|}{r^2} \frac{1}{\sqrt{r^2 - |w'|^2}} \Theta(r - |w'|). \quad (78)$$

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