Theory of laser-assisted electron momentum spectroscopy: Beyond the Volkov wave Born approximation

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Abstract. The \((e, 2e)\) spectroscopy of an atomic system at high impact energy and large momentum transfer is considered theoretically in the case of the presence of a laser field. The \((e, 2e)\) transition is supposed to take place due to electron-electron interaction. The incident electron is described by a Volkov wave. Several approximations for the three-body final state are formulated, which include the effects unaccounted by the Volkov wave Born approximation.

1. Introduction
The term “electron momentum spectroscopy” (EMS) [1, 2, 3, 4] usually refers to the \((e, 2e)\) method at high impact energy and large momentum transfer, when the latter is almost entirely absorbed by an ejected electron. EMS provides direct information on momentum distribution of electrons in various systems, ranging from atoms [5, 6] and molecules [7, 8, 9] to clusters [10] and solids [11, 12, 13]. This feature is due to the validity of the plane wave Born approximation (PWBA) for theoretical treatment of the EMS coincident differential cross sections (so-called momentum profiles). And when there are more or less appreciable effects beyond the scope of PWBA, one usually can take them into account by means of the distorted wave Born approximation (DWBA) (see, for instance, Weigold and McCarthy [3] and references therein) or, for instance, the 3C approach [14, 15].

Recently we have carried out the first theoretical consideration of the EMS process on an atomic system in the presence of laser radiation [16]. We found that the laser-assisted EMS method has a rich potential for investigating the laser-field effect on the target states even in
such situations where the laser electric-field amplitude is much weaker than a typical intra-atomic field. In particular, when the laser frequency is resonant to the frequency of the transition from the ground to the first excited target state, one observes characteristic EMS momentum profiles from the ground and excited states, populations of which depend on laser parameters, and the momentum profile from the excited state directly reflects the laser polarization. Our theoretical analysis has been carried out within the framework of the Volkov wave Born approximation (VWBA) which naturally generalizes the PWBA model to the case of the presence of a laser field. At the same time, in future laser-assisted EMS studies one might have a necessity for generalization of the models beyond PWBA. It is the aim of the present work to develop several such generalizations. Namely, we formulate analogs of the plane wave impulse approximation (PWIA), DWBA, and 3C approach in the case when the laser field is present.

The paper is organized as follows. In section 2, we deliver a general formulation of the problem and specify the $S$ matrix for the laser-assisted EMS process on an atomic target. Different models for the final state of the colliding system, which respectively determine different approximations to the $S$ matrix, are presented in section 3. Section 4 summarizes this work. Atomic units (a.u., $e = \hbar = m_e = 1$) are used throughout unless otherwise stated.

2. General formulation

We focus on the laser-assisted $(e,2e)$ reaction in an atomic system having only one active electron. High impact energy and large momentum transfer are assumed. The laser field switches on and off adiabatically at $t \to \mp \infty$, respectively, and is determined by the vector potential $A(t)$, which is treated in the dipole approximation. The laser intensity is supposed to be not so high as to induce any appreciable ionizing effect. The incident, scattered, and ejected electron energies and momenta are specified below by respectively $(E_0, \mathbf{p}_0)$, $(E_s, \mathbf{p}_s)$, and $(E_e, \mathbf{p}_e)$.

The $S$ matrix for the process under consideration can be presented as

$$ S = -i \int_{-\infty}^{\infty} dt \left\langle \Phi_{p_0 p_1}(\mathbf{r}_0, \mathbf{r}_1, t) \left| \frac{1}{r_{01}} \chi_{p_0}(\mathbf{r}_0, t) \psi_T(\mathbf{r}_1, t) \right. \right\rangle, $$

where $r_{01} = \mathbf{r}_0 - \mathbf{r}_1$. $\chi_{p_0}(\mathbf{r}_0, t)$ is a nonrelativistic Volkov wave [17, 18] describing the motion of the incident electron under the action of the laser field. $\psi_T(\mathbf{r}_1, t)$ is a wave function of the field-dressed target electron state. $\Phi_{p_0 p_1}(\mathbf{r}_0, \mathbf{r}_1, t)$ is the final scattering state of the colliding system embedded in a background laser field.

The incident Volkov wave solves the following Schrödinger equation (hereafter we use the velocity gauge):

$$ i \frac{\partial}{\partial t} \chi_{p_0}(\mathbf{r}_0, t) = \frac{1}{2} \left[ \mathbf{p}_0 + \frac{1}{c} A(t) \right]^2 \chi_{p_0}(\mathbf{r}_0, t). $$

Thus, we have (see, for instance, Ref. [19])

$$ \chi_{p_0}(\mathbf{r}_0, t) = \exp \left\{ i \left[ \mathbf{p}_0 \cdot \mathbf{r}_0 - \alpha(\mathbf{p}_0, t) - Et - \zeta(t) \right] \right\}, $$

where $E = p^2/2$ and

$$ \alpha(\mathbf{p}_0, t) = \frac{1}{c} \int_{-\infty}^{t} \mathbf{p}_0 \cdot A(t') dt', \quad \zeta(t) = \frac{1}{2c^2} \int_{-\infty}^{t} A^2(t') dt'. $$

The target wave function is a solution to the time-dependent Schrödinger equation

$$ i \frac{\partial}{\partial t} \psi_T(\mathbf{r}_1, t) = \left\{ \frac{1}{2} \left[ \mathbf{p}_1 + \frac{1}{c} A(t) \right]^2 + V(\mathbf{r}_1) \right\} \psi_T(\mathbf{r}_1, t), $$

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with the boundary condition

$$\psi_T(r_1, t \to -\infty) \to \exp(-i E_g t) \psi_g(r_1),$$

where $E_g$ and $\psi_g(r_1)$ are the energy and wave function of the undressed ground state of the target.

The wave function $\Phi_{p_p, p_e}(r_0, r_1, t)$ describes the motion of two outgoing electrons (scattered and ejected) in the field of the ionized target. It is given by the solution of the Schrödinger equation

$$\frac{i}{\hbar} \frac{\partial}{\partial t} \Phi_{p_p, p_e}(r_0, r_1, t) = H \Phi_{p_p, p_e}(r_0, r_1, t),$$

(5)

with the Hamiltonian

$$H = \frac{1}{2} \left[ \hat{p}_0 + \frac{1}{c} \mathbf{A}(t) \right]^2 + \frac{1}{2} \left[ \hat{p}_1 + \frac{1}{c} \mathbf{A}(t) \right]^2 + V(r_0) + V(r_1) + \frac{1}{r_{01}},$$

(6)

where $V(r) \to -1/r$ at $r \to \infty$, and the boundary condition

$$\Phi_{p_p, p_e}(r_0, r_1, t \to +\infty) \to \exp[-i(E_s + E_e)t] \Phi_{p_p, p_e}^{(-)}(r_0, r_1),$$

(7)

where $\Phi_{p_p, p_e}^{(-)}(r_0, r_1)$ is the final stationary state of the colliding system in the field-free case.

3. Final-state models

In this section, several approximations to the final state of the colliding system are formulated. Note in this connection that the VWBA model of [16] amounts to neglecting in (6) interactions of outgoing electrons with the ionized target and between each other, which yields

$$\Phi_{p_p, p_e}(r_0, r_1, t) = \chi_{p_p}(r_0, t) \chi_{p_e}(r_1, t).$$

(8)

In the field-free case, the Volkov wave reduces to the plane wave,

$$\chi_p(r, t) \to \exp[i(p \cdot r - Et)],$$

and hence VWBA reduces to PWBA.

3.1. Volkov wave impulse approximation

If in (6) we neglect the interactions between outgoing electrons and the ionized target, then we obtain

$$\Phi_{p_p, p_e}(r_0, r_1, t) = \chi_{p_s}(R_{01}, t) \varphi_{p_e}^{(-)}(r_{01}), \quad R_{01} = \frac{1}{2}(r_0 + r_1), \quad P_{se} = p_s + p_e, \quad p_{se} = \frac{1}{2}(p_s - p_e),$$

(9)

where

$$\chi_{p_s}(r_0, t) = \exp \{ i [P_{se} \cdot R_{01} - \alpha(P_{se}, t) - (E_s + E_e)t - 2\zeta(t)] \}$$

(10)

can be regarded as a Volkov wave describing the motion of the electron pair as a whole in the laser field, and $\varphi_{p_e}^{(-)}(r_{01})$ is an outgoing Coulomb wave which describes the relative motion of the scattered and ejected electrons. It is readily seen that in the field-free case the function (9) is given by

$$\Phi_{p_p, p_e}(r_0, r_1, t) = \exp[i(P_{se} \cdot R_{01} - (E_s + E_e)t)] \varphi_{p_e}^{(-)}(r_{01}),$$

which amounts to the PWIA model traditionally employed in the EMS studies (see, for instance, Weigold and McCarthy [3]).
3.2. Distorted-Volkov wave Born approximation
Neglecting in (6) the electron-electron interaction, we get
$$\Phi_{p_0,p_e}(r_0,r_1,t) = \psi_{p_0}^{(-)}(r_0,t)\psi_{p_e}^{(-)}(r_1,t). \quad (11)$$

The function \(\psi_{p_0}^{(-)}(r,t)\) describes the state of the outgoing electron under the combined action of the potential \(V(r)\) and the laser field. Finding its exact form is, in general, an intractable task. The following approximation can be useful:

$$\psi_{p}^{(-)}(r,t) = \exp \{ -i[\alpha(p,t) + Et + \zeta(t)] \} \psi_{p}^{(-)}(r), \quad (12)$$

where \(\psi_{p}^{(-)}(r)\) is a distorted wave in the potential \(V(r)\). When switching off the potential \(V(r)\), the function (12) gives a Volkov wave. And in the field-free case, it gives the distorted wave, thus yielding, in accordance with (11), the DWBA model.

3.3. 3C-Volkov function
In the field-free case, the 3C function [14] is an approximation to the exact three-body stationary wave function \(\Phi_{p_0,p_e}^{(-)}(r_0,r_1)\). It is a product of three Coulomb waves, or, more specifically,

$$\Phi_{3C}(r_0,r_1) = e^{-ip_{sec}r_{01}}\varphi_{p_0}^{(-)}(r_0)\varphi_{p_e}^{(-)}(r_1)\varphi_{p_e}^{(-)}(r_{01}), \quad (13)$$

where \(\varphi_{p_0}^{(-)}(r_{0(1)})\) is an outgoing Coulomb wave in the potential \(-1/r_{0(1)}\). It obeys correct asymptotic conditions at \(r_0, r_1,\) and \(r_{01} \to \infty\). One can incorporate the laser-field effect into the 3C model by replacing \(\exp(-iE_et)\varphi_{p_0}^{(-)}(r_0)\) and \(\exp(-iE_et)\varphi_{p_e}^{(-)}(r_1)\) with the so-called Coulomb-Volkov waves [20]. Such a replacement yields

$$\Phi_{p_0,p_e}(r_0,r_1,t) = \exp \{ -i[\alpha(P_{sec},t) + (E_s + E_e)t + 2\zeta(t)] \} \Phi_{3C}(r_0,r_1). \quad (14)$$

It can be noted that models (9) and (11) (the latter if the distorting potential is \(V(r) = -1/r\)) are particular cases of (14).

4. Summary
In this work, we have considered the laser-assisted EMS of an atomic system from a theoretical viewpoint. A general definition of the corresponding \(S\) matrix has been given that allows to take into account the dynamical effects beyond the VVBA approach. Several approximations to the \(S\) matrix, based on different models of the final three-charged-particle scattering state, have been formulated. These approximations are generalizations of the usual “field-free” ones to the situation where the laser field is present. They can be useful in theoretical treatments of laser-assisted EMS measurements, which are feasible in near future.

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