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Gauge dependence of the strong-field approximation: Theory vs. experiment for photodetachment of F^-

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Abstract

The dependence of the strong-field approximation on the gauge used for the description of the driving laser field is reviewed in connection with the choice of the initial bound state of the unperturbed atom or ion. Electron energy spectra are calculated for the various combinations of gauge and wave function and compared with experimental data for photodetachment of F^- by a circularly polarized laser field [B. Bergues, Y. Ni, H. Helm, I. Yu. Kiyan, Phys. Rev. Lett. 95 (2005) 263002]. If the laser intensity is considered a fitting parameter, then our length-gauge results reproduce the experimental results very well. In contrast, in velocity gauge no satisfactory fit can be obtained for any intensity.

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1. Introduction

This contribution presents an attempt to simulate recent experiments on above-threshold detachment (ATD) from F^- by a strong circularly polarized laser field [1]. Strong-field ionization of atoms and negatively charged ions is very well described by the single-active-electron approximation (SAEA), which reduces the dynamics to that of the most lightly bound electron in the presence of an optimized one-electron potential [2]. There are, of course, effects that owe their existence to electron–electron correlation; see, e.g. [3]. For example, proving the fact that the negative hydrogen ion has no excited bound states requires a many-electron framework [4]. But for the description of off-resonant multiphoton ionization a many-electron description is not needed. Within the SAEA, the strong-field approximation (SFA) or, as it is also often referred to, the Keldysh–Faisal–Reiss (KFR) theory [5–8] is particularly well suited to negative ions, owing to the absence of the Coulomb interaction between the detached electron and the atomic core. Even though arguably the SFA constitutes the backbone of the theory of laser–atom interaction, not too many quantitative comparisons of SFA results with experimental data have been put forward [9–11,1].

The SFA violates the gauge invariance afforded by an exact quantum-mechanical description. Hence, the two gauges that are commonly used – length gauge and velocity gauge – generally yield different answers. Moreover, using the SFA in the context of the SAEA to a many-electron atom, one has to approximate the one-electron wave function of the initial bound state. Different approximations will yield different results in different gauges. Few investigations have been published that attempt to answer the question of which gauge is better suited to the SFA [12].

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In this paper, we will first summarize various results concerning gauge aspects of the SFA [13,12]. Our version of the SFA has been laid out in Refs. [11,14,15]. Using this approach, we were able to simulate the ATD experiments with F^- and a linearly polarized laser field [16]. These data are also very well described [17] by the effective-range theory [18]. We have also predicted the behavior of the ATD rates for an elliptically polarized laser field [14,15]. Using these results, we will then simulate ATD of F^- by a strong circularly polarized laser field [1] and investigate how the results depend on the choice of gauge and the initial negative-ion wave functions.

2. Gauge aspects of the SFA

In this section, we will collect some general formulas and results regarding the gauge dependence of the SFA. We consider the transition amplitude from a bound state $|\psi_0(t)\rangle = |0\rangle \exp(\mathrm{i}I_\mathrm{p}t)$ to a continuum state $|\psi_\mathbf{p}(t)\rangle$ of the same binding potential $V(\mathbf{r})$ due to irradiation by a laser field with the electric field (in the long-wavelength approximation) $\mathbf{E}(t) = -\partial\mathbf{A}(t)/\partial t$. In the SFA, it can be written down in the two equivalent forms (see, e.g. [19]):

$$M_\mathbf{p} = \int \mathrm{d}t \left\langle \psi_\mathbf{p}^{(\mathrm{Volkov})}(t) | H_\mathrm{I}(t) | \psi_0(t) \right\rangle \tag{1a}$$

$$= \int \mathrm{d}t \left\langle \psi_\mathbf{p}^{(\mathrm{Volkov})}(t) | V | \psi_0(t) \right\rangle, \tag{1b}$$

where either the matter–field interaction

$$H_\mathrm{I}(t) = \begin{cases} +\mathrm{i}\frac{e}{m}\nabla\cdot\mathbf{A}(t) + \frac{e^2}{2m}\mathbf{A}(t)^2 & (\text{V gauge}) \\ -e\mathbf{r}\cdot\mathbf{E}(t) & (\text{L gauge}) \end{cases} \tag{2}$$

or the binding potential $V(\mathbf{r})$ is sandwiched between the Volkov state

$$\left\langle \mathbf{r} | \psi_\mathbf{p}^{(\mathrm{Volkov})}(t) \right\rangle = (2\pi)^{-3/2} \mathrm{e}^{-\mathrm{i}S_\mathbf{p}(t)} \begin{cases} \mathrm{e}^{\mathrm{i}\mathbf{p}\cdot\mathbf{r}} & (\text{V gauge}) \\ \mathrm{e}^{\mathrm{i}[\mathbf{p}-e\mathbf{A}(t)]\cdot\mathbf{r}} & (\text{L gauge}) \end{cases} \tag{3}$$

with drift momentum $\mathbf{p}$ and the field-free ground state. Both the matter–field interaction and the Volkov state, but not the field-free ground state, depend on the gauge employed, as shown. In the Volkov wave function (3), only the spatial part is gauge dependent, while the action

$$S_\mathbf{p}(t) = \frac{1}{2m}\int^t \mathrm{d}\tau [\mathbf{p} - e\mathbf{A}(\tau)]^2 \tag{4}$$

has the same form in either gauge. Of course, in length gauge where the vector potential vanishes, $\mathbf{A}(t)$ is short hand for $-\int^t \mathrm{d}\tau \mathbf{E}(\tau)$. The standard derivations of the SFA can be carried out in either length gauge or velocity gauge. The approximations that are introduced in doing so appear to be mathematically equivalent but actually amount to different approximations to the physics involved. This statement may sound strange but is proven by the fact that the amplitudes (1) yield different results when evaluated in different gauges. A third form of the ionization amplitude:

$$M_\mathbf{p} = -\int \mathrm{d}t \left\langle \psi_\mathbf{p}^{(\mathrm{Volkov})}(t) | \psi_0(t) \right\rangle \times \begin{cases} \left(\frac{1}{2m}[\mathbf{p} - e\mathbf{A}(t)]^2 + I_\mathrm{p}\right) & (\text{L gauge}) \\ \left(\frac{1}{2m}\mathbf{p}^2 + I_\mathrm{p}\right) & (\text{V gauge}), \end{cases} \tag{5}$$

can be obtained from Eq. (1b) by writing $V = [-1/(2m)\nabla^2 + V] + 1/(2m)\nabla^2$ and applying the first term to the right and the second term to the left. For general gauge considerations, the form (1b) is particularly useful, since the gauge dependence is confined to the Volkov state. For numerical calculations, the form (1a) has the advantage that it requires only knowledge of the ground-state wave function, which is tabulated, and not of the binding potential $V(\mathbf{r})$ that generates the former.

We will discuss the gauge dependence of the amplitudes (1) based on their evaluation by the saddle-point approximation (SPA). Hence, our conclusions must be applied with some care outside the tunneling regime. However, all explicit results presented in the subsequent sections are derived by numerical computation and do not depend on the SPA. In the SPA, the integral over time in the amplitudes (1) can be approximately carried out by restricting it to the vicinity of those times t where the action $S_\mathbf{p}(t) + I_\mathrm{p}t$ is stationary. They are determined by the solutions $t = t_s$ of the equation

$$[\mathbf{p} - e\mathbf{A}(t)]^2 = \mathbf{p}_\perp^2 + [\mathbf{p}_\parallel - e\mathbf{A}(t)]^2 = -2mI_\mathrm{p}, \tag{6}$$

which holds in either gauge. The SPA to the ionization amplitude in the form (1b) then reads

$$M_\mathbf{p} = \sum_s V_{\mathbf{p}s} \sqrt{\frac{2\pi\mathrm{i}}{\mathbf{E}(t_s)\cdot[\mathbf{p} - e\mathbf{A}(t_s)]}} \mathrm{e}^{\mathrm{i}[S_\mathbf{p}(t_s) + I_\mathrm{p}t_s]}, \tag{7}$$

where the sum is over those times t_s with $\mathrm{Im}\,t_s > 0$; see, e.g. [19]. In this form, the gauge dependence is entirely contained in the form factors

$$V_{\mathbf{p}s} = \begin{cases} \langle \mathbf{p} | V | 0 \rangle & (\text{V gauge}) \\ \langle \mathbf{p} - e\mathbf{A}(t_s) | V | 0 \rangle & (\text{L gauge}) \end{cases}. \tag{8}$$

The form factor is the Fourier transform of the product of the binding potential $V(\mathbf{r})$ times the ground-state wave function. According to (8), in velocity gauge it is evaluated at the drift momentum $\mathbf{p}$ while in length gauge it is taken at the instantaneous momentum $\mathbf{p} - e\mathbf{A}(t_s)$ at the tunneling time t_s. Owing to the saddle-point equation (6), this latter momentum is complex, even purely imaginary, if the drift momentum has no component $\mathbf{p}_\perp$ perpendicular to the laser polarization. For a zero-range binding potential and an s ground state, $V_{\mathbf{p}s}$ does not depend on $\mathbf{p}$. So, in this case, the form factor and thereby the entire ionization amplitude do not depend on the gauge. For the case of H^- and linear polarization, this was already observed by Dörr et al. [20].

According to the derivations of the SFA, the initial state $|0\rangle$ is an eigenstate (normally the ground state) of the