Gauge-invariant relativistic strong-field approximation

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The problem of the choice of gauge in the relativistic strong-field approximation (SFA) is analyzed. The main motivation is to obtain a relativistic ionization amplitude in the SFA which in the nonrelativistic limit coincides with the conventional well-accepted results of the SFA in the length gauge. A gauge-invariant formulation of the SFA is derived which is applicable both in the nonrelativistic as well as in the relativistic regime of laser-induced strong-field ionization phenomena. The gauge invariance is achieved by means of employment of an eigenstate of the physical energy operator for the initial atomic state. As an example, a comparison of predictions of the gauge-invariant theory with conventional SFA results in the radiation gauge is given for above-threshold ionization in the relativistic regime.

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INTRODUCTION

The strong-field approximation (SFA) is one of a few nonperturbative analytical approaches in the field of strong-laser-radiation interaction with atomic systems [1]. Stemming from the heuristic Keldysh approximation [2], it has been developed as a rigorous theory based on a specific expansion of the exact Green's function, treating nonlinear ionization in the nonrelativistic [3,4] as well as in the relativistic domain [5,6]. The SFA provides a unified description of the strong-field ionization phenomena in the multiphoton and tunneling regimes. It proved to be very fruitful in describing and predicting features of above-threshold ionization (ATI) and high-order-harmonic generation (HOHG) phenomena [7,8]. A quantum orbit theory has been developed based on the SFA which provides a detailed insight into ATI and HOHG phenomena [7,9–11].

The SFA is not a gauge-invariant theory, as was pointed out a long time ago [12]. Moreover, discrepancies between the results of different gauges can be significant [13]. It is accepted that the SFA, being an approximate treatment that neglects the influence of the atomic potential for the ionized electron, cannot be gauge invariant, in contrast to the gauge-invariant exact transition amplitude. Therefore, specific investigations are necessary to choose an appropriate gauge for the treatment of processes within the SFA. This is done for the nonrelativistic regime of interaction. Thus, recently for the ionization of negative ions with a short-range binding potential, a comparison has been carried out between results of the nonrelativistic SFA in the length and velocity gauge, and the solution of the time-dependent Schrödinger equation [14]. It has been shown that the velocity and length gauges can yield qualitatively different results. The solution of the time-dependent Schrödinger equation in the considered case is close to the result of the SFA in the length gauge [14]. An exact solution for the ionization from a zero-range effective potential exists [15], which is also in favor of the SFA with the length gauge. The same can be said about experimental results, for instance, the experiment on above-threshold detachment for the negative F^- ion [16]. Another intuitive argument in favor of the length gauge is given in [17]. In the length gauge large distances become important in the calculation of the transition matrix element, and only at large distances can one neglect Coulomb interactions in the exact wave function. Therefore, a conclusion has been reached that in the nonrelativistic domain the SFA provides an adequate description of the ionization phenomena in the length gauge.

In the relativistic regime, detailed investigations comparing the SFA in different gauges with the solution of the time-dependent Dirac and Klein-Gordon equations or experimental results are still missing. We are faced with the problem of choosing the gauge for the SFA in the relativistic regime, and we consider this problem in this paper. To have a unified approach in the nonrelativistic as well as in the relativistic regime, we proceed in the following way. Accepting that in the nonrelativistic regime the length gauge has turned out to be the proper gauge for the SFA, we develop a nonrelativistic gauge-invariant amplitude which coincides with the conventional SFA result in the length gauge. Then in the next step we apply the corresponding procedure in the relativistic regime. As a result we derive a relativistic SFA wave function which is consistent with the well-accepted nonrelativistic SFA results, that is, with the nonrelativistic SFA results in the length gauge as well as with the intuitive physical arguments of [14].

Let us recall the intuitive physical arguments of [14] justifying the use of the length gauge in the SFA. This will explain the ansatz that we apply later to solve the wave equation. The main essence of the SFA is known to be the following two assumptions: (1) the influence of the Coulomb field of the atomic core on the dynamics of the ionized electron is small in comparison with the laser field, and (2) the influence of the laser field on the initial bound state of the atomic system is negligible. To realize this physical content

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of the SFA, the exact wave function in the exact transition amplitude is replaced by the Volkov wave function which describes the electron in the laser field alone [18,19].

Thus, starting with the exact expression for the ionization amplitude we have [7]

$$M_{\mathbf{p}} = -i\int_{-\infty}^{\infty} d\tau \langle \Psi_{\mathbf{p}}(\tau)|H_{int}(\tau)|\Psi_0(\tau)\rangle, \quad (1)$$

where $\Psi_{\mathbf{p}}(\tau)$ is the exact wave function corresponding to the continuum state in the atomic potential in the remote future, when the laser field is adiabatically switched off, $\Psi_0(\tau)$ is the initial bound-state wave function in the remote past, when the laser field is adiabatically switched on, and H_{int} is the laser-atom interaction Hamiltonian: $H_{int}=\mathbf{E}\cdot\mathbf{r}\equiv H_I^{(l)}$ in the length gauge or $H_{int}=\mathbf{A}\cdot\hat{\mathbf{p}}/c+\mathbf{A}^2/2c^2\equiv H_I^{(v)}$ in the velocity gauge, with the laser electric field $\mathbf{E}$, the vector potential $\mathbf{A}$, the momentum operator $\hat{\mathbf{p}}$, and the speed of light c. Atomic units are used throughout the paper. Then, replacing the exact wave function $\Psi_{\mathbf{p}}(\tau)$ in Eq. (1) with the Volkov wave function $\Psi_{\mathbf{p}}^{(V)}(\tau)$ [18,19], yields the amplitude in the SFA,

$$M_{\mathbf{p}} = -i\int_{-\infty}^{\infty} d\tau \langle \Psi_{\mathbf{p}}^{(V)}(\tau)|H_{int}(\tau)|\Psi_0(\tau)\rangle. \quad (2)$$

The latter indicates the following approximate physical picture of the interaction dynamics [14]: up to the moment $t<\tau$ the electron is in the bound state of the atom $\Psi_0(t)$ not perturbed by the laser field, while at a time $t=\tau$ the laser-atom interaction via $H_{int}(t)$ causes the transition of the electron to an ionized state which is a pure Volkov state of the electron in the laser field. Only the length gauge is consistent with this picture, as argued in [14], because only in the length gauge is the state $\Psi_0(t)$ at the moment $t<\tau$, when the laser field is already switched on, the eigenstate of the *physical* energy operator of the free atom [20],

$$\hat{\mathcal{E}} = (\hat{\mathbf{p}} + \mathbf{A}/c)^2/2 + V(\mathbf{r}). \quad (3)$$

Notice that $\Psi_0(\tau)$ is the eigenstate of the free atomic Hamiltonian $H_0=\hat{\mathbf{p}}^2/2+V(\mathbf{r})$, with the atomic binding potential $V(\mathbf{r})$, and in the length gauge the vector potential disappears, $\mathbf{A}=\mathbf{0}$.

The exact amplitude (1) is gauge invariant while the amplitude (2) in the SFA is not. Thus, the conventional SFA provides different results for different gauges. This can be understood as that in different gauges the above-mentioned replacement of the exact wave function by the Volkov solution corresponds in reality to different physical approximations, and that only the length gauge corresponds to the physical requirements of the SFA as formulated in the two points above.

At this point let us also recall a similar problem of gauge dependence of perturbative bound-bound atomic transitions in a laser field (see, e.g., [20–29]). In short it is the following. In the perturbative nonrelativistic treatment of atomic transitions, the total Hamiltonian is usually split into two parts $H=H_0+H_{int}$, the free atomic Hamiltonian H_0 and the interaction Hamiltonian H_{int}. When the free atomic Hamiltonian H_0 is taken as an unperturbed Hamiltonian and the perturbed wave function is expanded in terms of eigenstates of H_0, then the transition probabilities are expressed via matrix elements of the interaction Hamiltonian which is equal to either $H_I^{(l)}$ (length gauge) or $H_I^{(v)}$ (velocity gauge). These matrix elements in general are different for nonresonant transitions, yielding gauge-dependent results. A principal solution of this problem has been proposed in [22] by means of choosing a specific basis for the initial and final states of the atom. A statement is made that the physical transition of an atomic system in a laser field is represented by a transition between the eigenstates of the *physical* energy operator $\hat{\mathcal{E}}$ of Eq. (3) and not between eigenstates of the unperturbed Hamiltonian H_0 [20]. The perturbation theory based on the expansion in terms of eigenstates of the physical energy operator $\hat{\mathcal{E}}$ proved to be gauge invariant and yields gauge-invariant transition amplitudes [29]. Nevertheless, there is an important difference between the SFA and the perturbative atomic transitions. In the latter case if the laser field is adiabatically switched on and off, then the gauge dependence of the transition amplitude disappears [26,27]. Meanwhile, the SFA with an adiabatically switching laser field gives gauge-dependent results, which, as explained above, is an indication of the fact that the resultant approximations are physically different in the different gauges.

In this paper we employ the physical energy operator eigenstates within the SFA ideology. We begin our discussion with the nonrelativistic Schrödinger equation (Sec. I), introduce a modified SFA ansatz, then generalize our treatment for the relativistic regimes based on the Klein-Gordon equation (Sec. II) and the Dirac equation (Sec. III), and give our conclusion in the final section.

I. THE NONRELATIVISTIC REGIME

We consider the ionization process of an atomic system by an arbitrarily polarized laser field. Further, the single-active-electron approximation is applied, i.e., the interaction of the set free electron with the ionic core plus bound electrons is represented by a static effective atomic short-range potential.

As is known the ionization dynamics is well described by the Schrödinger equation for the wave function of the active electron Ψ for laser intensities up to 10^{16} W/cm^2 at a sub-optical laser wavelength (see, e.g., [30]):

$$i\partial_t\Psi = [(\hat{\mathbf{p}} + \mathbf{A}/c)^2/2 + V - \phi]\Psi, \quad (4)$$

where ϕ and $\mathbf{A}$ are the scalar and the vector potential of the laser field, respectively, and V is the atomic short-range potential. We do not specify the gauge at this point. As usual in the nonrelativistic case the dipole approximation is applied since the characteristic length of the electron motion in this regime is much smaller than the wavelength of the laser.

By solving the equation of motion (4) we will make the standard assumptions of the SFA [1]. That is, the influence of the laser field on the ground state is neglected, particularly the Stark shift and the depletion of the atomic ground state. The contributions of all other bound states are assumed to be negligible. Further, the ionized electron is assumed to be only affected by the laser field, not by the potential of the atomic core.

We represent the time-dependent wave function of the atom in the laser field in an intermediate moment t of the interaction as a superposition of the atomic unperturbed bound state and the ionized wave:

$$\Psi(t) = \Psi_0(t) + \tilde{\Psi}(t), \tag{5}$$

where $\Psi_0(t)$ describes the electron in the bound state and $\tilde{\Psi}(t)$ the ionized electron. The ionized wave should disappear $\tilde{\Psi}(t) \to 0$ before the interaction $t \to -\infty$. According to the SFA assumption that the bound state is not disturbed by the laser field, $\Psi_0(t)$ should be the eigenstate of the physical energy operator of the free atom with a negative eigenvalue ε_0:

$$[(\hat{\mathbf{p}} + \mathbf{A}/c)^2/2 + V]\Psi_0 = \varepsilon_0 \Psi_0. \tag{6}$$

At an intermediate moment of the interaction $\mathbf{A}(t) \neq \mathbf{0}$ therefore the physical energy operator does not coincide with the atomic Hamiltonian $H_0 = \hat{\mathbf{p}}^2/2 + V(\mathbf{r})$. The ansatz of Eq. (5) corresponds to the intuitive picture represented in the Introduction.

The part of the wave function describing the ionization can be in general represented via an expansion in terms of Floquet eigenstates of the total Hamiltonian. Then we will have the following ansatz for the total wave function:

$$\Psi(\mathbf{r},t) = \Psi_0(\mathbf{r},t) + \sum_n c_n(t)\Psi_n(\mathbf{r},t), \tag{7}$$

where $\Psi_0(\mathbf{r},t) = \Phi_0(\mathbf{r},t)\exp(-i\varepsilon_0 t)$, and n indicates the quantum numbers of the Floquet states. The Floquet eigenstates $\Psi_n(t) = \exp(-i\varepsilon_n t)\Phi_n(\mathbf{r},t)$ with the quasienergy ε_n and the periodic quasienergy wave function $\Phi_n(\mathbf{r},t)$ (the quasienergy wave function is periodic with the laser field period) are the eigenstates of the total Hamiltonian

$$i\partial_t \Psi_n = [(\hat{\mathbf{p}} + \mathbf{A}/c)^2/2 + V - \phi]\Psi_n. \tag{8}$$

The orthonormal set of Floquet eigenstates constitutes the set of possible final states of the system. Later, the exact Floquet eigenstates will be replaced by the Volkov states using the second assumption of the SFA that the ionized state is mainly governed by the laser field.

The Schrödinger equation (4) with the ansatz (7) yields the following expression for the coefficients $c_n(t)$:

$$c_n(t) = i\int_{-\infty}^{t} e^{-i\varepsilon_0\tau} d\tau \int d\mathbf{r}\, \Psi_n^*(\mathbf{r},\tau)(\phi + i\partial_\tau)\Phi_0(\mathbf{r},\tau). \tag{9}$$

In the dipole approximation the vector potential is only time dependent, $\mathbf{A} = \mathbf{A}(t)$, which allows one to solve Eq. (6) exactly and to find the wave function of the bound state of the electron

$$\Phi_0(\mathbf{r},t) = \phi_0(\mathbf{r})\exp[-i\mathbf{A}(t)\cdot\mathbf{r}/c] \tag{10}$$

where $\phi_0(\mathbf{r})$ is the eigenstate of the Hamiltonian H_0. Then, inserting the expression for the electron initial state (10) into Eq. (9), using the electric field definition $\mathbf{E}(t) = -\boldsymbol{\nabla}\phi - \partial_t \mathbf{A}(t)/c$ as well as the fact that the only time dependence of the electric field results in a linear space dependence of ϕ, and taking into account that at $t \to -\infty$ the ionized wave disappears, yields for the transition amplitude

$$c_n(t) = -i\int_{-\infty}^{t} d\tau \langle \Psi_n(\tau)|\mathbf{E}(\tau)\cdot\mathbf{r}|\Psi_0(\tau)\rangle. \tag{11}$$

This formula for the transition amplitude is derived for an arbitrary gauge. It is still exact, and therefore gauge invariant, and is expressed via the exact Floquet eigenstate of the total Hamiltonian. Notice that the expression of Eq. (11) coincides with the corresponding coefficients describing ionization amplitudes in the nonrelativistic treatment of [17]; see the time integral of Eq. (A3) in [16]. In fact, both expressions are gauge invariant and are identical in the length gauge.

Now we can apply the SFA, which from the mathematical point of view is reduced to replacing the exact Floquet eigenstate of the total Hamiltonian Ψ_n by the Floquet eigenstate of the electron only in the laser field, i.e., by the nonrelativistic Volkov wave function $\Psi_{\mathbf{p}}^V$ with drift momentum $\mathbf{p}$. The latter satisfies the equation

$$i\partial_t \Psi_{\mathbf{p}}^V = [(\hat{\mathbf{p}} + \mathbf{A}/c)^2/2 - \phi]\Psi_{\mathbf{p}}^V. \tag{12}$$

The explicit expression for the nonrelativistic Volkov wave function in the velocity gauge is

$$\breve{\Psi}_{\mathbf{p}}^V(\mathbf{r},t) = \frac{1}{\sqrt{(2\pi)^3\mathcal{V}}}\exp\left[i\mathbf{p}\cdot\mathbf{r} + \frac{i}{2}\int_t^{\infty} d\tau\left(\mathbf{p} + \frac{\breve{\mathbf{A}}(\tau)}{c}\right)^2\right], \tag{13}$$

which at the $t \to \infty$ limit yields a plane wave with momentum $\mathbf{p}$, interaction volume $\mathcal{V}$, and

$$\breve{\mathbf{A}}(t) \equiv -c\int \mathbf{E}(t)dt. \tag{14}$$

By a corresponding gauge transformation the explicit form of the Volkov wave function can be easily obtained in any gauge.

The amplitude $M_{\mathbf{p}}$ for ATI yielding one electron with momentum $\mathbf{p}$ is given by

$$M_{\mathbf{p}} = \lim_{t\to\infty} c_{\mathbf{p}}(t). \tag{15}$$

Finally, from Eq. (11) we obtain for the ionization amplitude in the SFA

$$M_{\mathbf{p}} = -i\int_{-\infty}^{\infty} d\tau \langle \Psi_{\mathbf{p}}^V(\tau)|\mathbf{E}(\tau)\cdot\mathbf{r}|\Psi_0(\tau)\rangle. \tag{16}$$

We again underline that the initial state $\Psi_0(t)$ is determined by Eq. (10) as an eigenstate of the physical energy operator. The Volkov state is also an eigenstate of this operator.

We can derive a more convenient expression for the transition amplitude making the time integration by parts in Eq. (9) with the Volkov wave function and using the complex conjugate of Eq. (13):

$$M_{\mathbf{p}}(t) = -i\int_{-\infty}^{\infty} d\tau \int d\mathbf{r}\, \Psi_0(\mathbf{r},\tau)\{\varepsilon_0 - [\hat{\mathbf{p}} - \mathbf{A}(\tau)/c]^2/2\} \times \Psi_{\mathbf{p}}^{V*}(\mathbf{r},\tau). \tag{17}$$

Then, the transition amplitude reads

$$M_{\mathbf{p}} = -i\int_{-\infty}^{\infty} d\tau \langle \Psi_{\mathbf{p}}^{V}(\tau)|V|\Psi_0(\tau)\rangle = -i\int_{-\infty}^{\infty} dt' \left\langle \mathbf{p} + \frac{\breve{\mathbf{A}}(t')}{c}|V|0 \right\rangle e^{iS(\mathbf{p},t,t')}, \tag{18}$$

where $\langle \mathbf{p}|V|0\rangle$ is the matrix element of the atomic potential, $S(\mathbf{p},t,t')=\int_t^{t'} d\tau\{[\mathbf{p}+\breve{\mathbf{A}}(\tau)/c]^2/2+I_p\}$ is the quasiclassical action, and I_p is the ionization potential.

The amplitude expressions of Eqs. (16) and (18) are valid for any gauge and are gauge invariant. Moreover, they coincide with the ionization amplitude derived by the conventional SFA in the length gauge which, as already mentioned in the Introduction, give the adequate physical description of the ionization process in the nonrelativistic regime [7].

II. THE KLEIN-GORDON REGIME

If spin effects [31] are not of significance then the dynamics of the ionized electron may be described by the Klein-Gordon equation for the wave function $\Psi(x)$:

$$[(i\partial^{\mu} + A^{\mu}/c + g^{\mu 0}V/c)^2 - c^2]\Psi(x) = 0 \tag{19}$$

with $\mu\epsilon\{0,1,2,3\}$. $A^{\mu}=(\phi,\mathbf{A})$ is the vector potential of an arbitrary polarized laser field (the gauge is not fixed), $x=(ct,x,y,z)$ the time-space coordinates, $k^{\mu}=(\omega/c,0,0,k)$ its wave vector, $\omega=ck$ its angular frequency, and $g^{\mu\nu}$ the metric tensor.

Analogous to the nonrelativistic case, we apply the ansatz (7) for the wave function. The wave function of the initial state $\Psi_0=\Phi_0\exp(-i\int\varepsilon_0 d\tau)$ is an eigenstate of the physical energy

$$[(\varepsilon_0 - V)^2/c^2 - (\hat{\mathbf{p}} + \mathbf{A}/c)^2 - c^2]\Phi_0(x) = 0. \tag{20}$$

We assume that the atom is initially in the ground state with the ground-state energy ε_0. The Floquet eigenstates $\Psi_n(t)$ of the total Hamiltonian satisfy the Klein-Gordon equation (19).

Inserting Eq. (7) in Eq. (19) now yields

$$\sum_n [\ddot{c}_n(t)\Psi_n(x) + 2\dot{c}_n(t)\partial_t\Psi_n(x) + 2i(V-\phi)\dot{c}_n(t)\Psi_n(x)] = [(i\partial_t + \phi - V)^2 - (\varepsilon_0 - V)^2]\Psi_0(x), \tag{21}$$

where the overdot indicates a time derivative. Projecting Eq. (21) to a state Ψ_k, integrating by time, and using the orthonormality relation

$$\int d\mathbf{r}[i(\Psi_k^*\partial_t\Psi_n - \Psi_n\partial_t\Psi_k^*) - 2(V-\phi)\Psi_k^*\Psi_n] = \delta_{kn} \tag{22}$$

yields for the transition amplitude

$$M_n = i\int d^4x\, \Psi_n^*(x)\{-\partial_t^2\Phi_0(x) + 2i(\varepsilon_0 + \phi - V)\partial_t\Phi_0(x) + [i\dot{\varepsilon}_0 + i\partial_t\phi - 2\phi(V-\varepsilon_0) + \phi^2]\Phi_0(x)\} \times \exp\left(-i\int \varepsilon_0 d\tau\right). \tag{23}$$

Transition amplitudes in the SFA are obtained by replacing the exact Floquet eigenstates $\Psi_n(x)$ in Eq. (23) by the Volkov wave function of the electron in a laser field $\Psi_{\mathbf{p}}^{V}(x)$:

$$M_{\mathbf{p}} = i\int d^4x\, \Psi_{\mathbf{p}}^{V*}(x)\{-\partial_t^2\Phi_0(x) + 2i(\varepsilon_0 + \phi - V)\partial_t\Phi_0(x) + [i\dot{\varepsilon}_0 + i\partial_t\phi - 2\phi(V-\varepsilon_0) + \phi^2]\Phi_0(x)\} \times \exp\left(-i\int \varepsilon_0 d\tau\right). \tag{24}$$

The Volkov wave function is described by the Klein-Gordon equation of the electron in a laser field

$$[(i\partial^{\mu} + A^{\mu}/c)^2 - c^2]\Psi_{\mathbf{p}}^{V}(x) = 0. \tag{25}$$

In the velocity gauge it reads [1]

$$\breve{\Psi}_{\mathbf{p}}^{V}(x) = \frac{1}{\sqrt{2\mathcal{V}\varepsilon_{\mathbf{p}}}}\exp\left(-ip\cdot x + i\int_{\eta}^{\infty} d\tilde{\eta}\frac{[\mathbf{p} + \breve{\mathbf{A}}(\tilde{\eta})/2c]\cdot\breve{\mathbf{A}}(\tilde{\eta})/c}{k\cdot p}\right), \tag{26}$$

with $\varepsilon_{\mathbf{p}}=\sqrt{c^2\mathbf{p}^2+c^4}$, $\eta=k^{\mu}x_{\mu}\equiv k\cdot x$ the phase of the laser field, and $\breve{\mathbf{A}}(\eta)$ defined in Eq. (14).

Integration by parts of Eq. (23), taking into account Eq. (25), reduces the ionization amplitude to the following expression:

$$M_{\mathbf{p}} = i\int_{-\infty}^{\infty} d\tau\langle\Psi_{\mathbf{p}}^{V}(\tau)|V^2 - 2iV\partial_t - 2\phi V|\Psi_0(\tau)\rangle. \tag{27}$$

The expressions for the transition amplitude of Eqs. (24) and (27) are valid for any gauge. It is easy to verify that the transition amplitude of Eqs. (24) and (27), along with the Klein-Gordon equation (19) and the equations for the initial and final states (20) and (25), are invariant under the gauge transformation

$$\Psi_0' = e^{if(x)}\Psi_0, \quad \Psi_{\mathbf{p}}^{V\prime} = e^{if(x)}\Psi_{\mathbf{p}}^{V},$$

$$\mathbf{A}' = \mathbf{A} - \nabla f(x), \quad \phi' = \phi + \partial_t f(x). \tag{28}$$

For more simplification of the expression for the transition amplitude we need an explicit expression for the initial state $\Phi_0(x)$. It is an eigenstate of the physical energy operator and obeys Eq. (20), which cannot be solved exactly. Nevertheless, one may simplify the equation for the energy eigenstate, using a small parameter: the ratio of the atomic velocity $v_a=Zc\alpha$ to the velocity of light, where α is the fine-structure constant and Z the ion charge. This approximation cis easier to perform in the gauge where the canonical momentum operator $\hat{\mathbf{p}}$ does not differ significantly from the kinetic momentum operator. In the nonrelativistic limit this is the length gauge, where the canonical momentum operator coincides with the kinetic one, while in the relativistic case, the Göppert-Mayer gauge (the relativistic generalization of the length gauge applicable for plane-wave fields) has this kind of property.

In fact, let us employ the Göppert-Mayer gauge [1,32] in Eq. (20):

$$\tilde{\phi} = -\mathbf{E}\cdot\mathbf{r}, \quad \tilde{\mathbf{A}} = -\frac{\mathbf{k}}{\omega}(\mathbf{E}\cdot\mathbf{r}). \tag{29}$$

Consequently, we obtain the following equation for the wave function in the Göppert-Mayer gauge $\tilde{\Phi}_0(x)$:

$$\left[\frac{[\varepsilon_0 - V]^2}{c^2} - \left(\hat{\mathbf{p}} - \frac{\mathbf{k}}{\omega}\cdot(\mathbf{E}\cdot\mathbf{r})\right)^2 - c^2\right]\tilde{\Phi}_0(x) = 0. \tag{30}$$

Let us estimate the different terms in Eq. (30) for a hydrogenlike atom and a moderately relativistic laser field with a relativistic parameter $\xi \equiv A_0/c^2 \sim 1$. Neglecting the Stark shift of the atomic ground state, its energy can be approximated by $\varepsilon_0 \approx c^2 - I_p$. Estimating x, z and p_x, p_z as the bound-electron coordinate and momentum in the laser polarization and propagation direction, respectively, yields $x \sim z \sim 1/Zc\alpha \sim 1/\sqrt{I_p}$ and $p_x \sim p_z \sim Zc\alpha \sim \sqrt{I_p}$. The vector potential estimation gives $\tilde{A} \approx Ex \sim \xi\omega/Z\alpha$. The ratio $\tilde{A}/cp_x \sim \xi\omega/I_p$, which is of order 10^{-3} at $\xi \sim 1$, $\omega \approx 1$ eV, and $Z^2 \approx 10$. Therefore, the kinetic momentum approximation by the canonical one is justified. To be more precise, for a hydrogenlike atom like B^{4+} with ionization potential $I_p = 12.5$ a.u., a laser field with $\xi = 0.5$ and suboptical angular frequency $\omega = 0.05$ a.u., we obtain for the terms of Eq. (30) the estimates

$$O(V/c^2) \sim I_p/c^2 \sim 7\times 10^{-4},$$

$$O(p^2/c^2) \sim I_p/c^2 \sim 7\times 10^{-4},$$

$$O(2(\mathbf{E}\cdot\mathbf{r})p_z/c^3) \sim \xi\omega/c^2 \sim 10^{-6},$$

$$O((\mathbf{E}\cdot\mathbf{r})^2/c^4) \sim \xi^2\omega^2 I_p/c^2 \sim 4\times 10^{-7}. \tag{31}$$

Consequently, the equation for the ground-state wave function in the Göppert-Mayer gauge reduces to the nonrelativistic unperturbed Schrödinger equation for the electron in the atomic potential $V(\mathbf{r})$:

$$(\hat{\mathbf{p}}^2/2 + V + I_p)\tilde{\Phi}_0(x) = 0. \tag{32}$$

Thus, the initial wave function can be approximated by the nonrelativistic ground-state wave function

$$\tilde{\Phi}_0(x) = \phi_0(x)\exp[-i(c^2 - I_p)t]/\sqrt{2(c^2 - I_p)}. \tag{33}$$

In any other gauge the wave function of the initial state is derived from $\tilde{\Phi}_0(x)$ by means of the gauge transformation.

Having derived an approximate expression for the initial-state wave function (33), we can proceed by simplifying the ionization amplitude. The expression for the ionization amplitude of Eq. (24) reduces to

$$M_{\mathbf{p}} = i\int d^4x\, \Psi_{\mathbf{p}}^{V*}(x)[(\mathbf{E}\cdot\mathbf{r})^2 - 2(c^2 - I_p + V)\mathbf{E}\cdot\mathbf{r} - i\omega\mathbf{E}'\cdot\mathbf{r}]\Psi_0(x) \approx -2ic^2\int d^4x\, \Psi_{\mathbf{p}}^{V*}(x)(\mathbf{E}\cdot\mathbf{r})\Psi_0(x), \tag{34}$$

where the prime denotes a derivative by the laser phase.

Likewise, the ionization amplitude of Eq. (27) reduces to

$$M_{\mathbf{p}} = i\int_{-\infty}^{\infty} d\tau\langle\Psi_{\mathbf{p}}^{V}(\tau)|V^2 - 2V(c^2 - I_p) + 2(\mathbf{E}\cdot\mathbf{r})V|\Psi_0(\tau)\rangle \approx -2ic^2\int_{-\infty}^{\infty} d\tau\langle\Psi_{\mathbf{p}}^{V}(\tau)|V|\Psi_0(\tau)\rangle. \tag{35}$$

The last expression for the amplitude after the transformation of coordinates $(t,\mathbf{r}) \to (\eta,\mathbf{r})$ can be written in the following form:

$$M_{\mathbf{p}} = -i\lim_{\eta\to\infty}\int_{-\infty}^{\infty} d\eta'\frac{c^2\exp[iS(\mathbf{p},\eta,\eta')]}{\sqrt{\varepsilon_{\mathbf{p}}(c^2 - I_p)\omega}} \times \left\langle \mathbf{p} + \frac{\breve{\mathbf{A}}(\eta')}{c} - \frac{\mathbf{k}}{\omega}(\varepsilon_{\mathbf{p}} + I_p - c^2)|V|0\right\rangle, \tag{36}$$

where $S(\mathbf{p},\eta,\eta') = \int_\eta^{\eta'} d\tilde{\eta}[\tilde{\varepsilon}_{\mathbf{p}}(\tilde{\eta}) - c^2 + I_p]/\omega$ is the quasiclassical action and the electron energy in the field is given by

$$\tilde{\varepsilon}_{\mathbf{p}}(\eta) = \varepsilon_{\mathbf{p}} + \frac{\omega}{k\cdot p}\left(\mathbf{p} + \frac{\breve{\mathbf{A}}(\eta)}{2c}\right)\cdot\frac{\breve{\mathbf{A}}(\eta)}{c}. \tag{37}$$

The ionization amplitudes in the gauge-invariant SFA of Eqs. (34)–(36) differ from the standard SFA result in the velocity gauge by an additional term of $\breve{\mathbf{A}}(\eta)/c$ in the argument of the matrix element $\left\langle \mathbf{p} + \frac{\breve{\mathbf{A}}(\eta')}{c} - \frac{\mathbf{k}}{\omega}(\varepsilon_{\mathbf{p}} + I_p - c^2)|V|0\right\rangle$. Accordingly, the ratio of the preexponential factors for the gauge-invariant SFA to the conventional SFA is of the order $\sim p_x/(p_x + \breve{A}) \sim \sqrt{U_p/I_p} \sim 1/\gamma$, because from the approximate saddle point condition $(p_x + A)^2 = 2I_p$, whereas p_x is of the order of $\sqrt{U_p}$, where $U_p = \langle A^2/2\rangle$, $\kappa = \sqrt{2I_p}$; $\gamma \equiv \sqrt{I_p/2U_p}$ is the Keldysh parameter, and can be small in the relativistic tunneling regime.

In fact, the region of parameters ξ and Z where the tunneling ionization regime of a hydrogenlike ion takes place is shown in Fig. 1 as a shaded region. This region is defined by two conditions; the first is $\gamma < 1$,

$$\xi > \sqrt{2I_p/c^2}, \tag{38}$$

and the second that the laser intensity must be not so large as to sweep the atomic electron over the barrier [33], i.e.,

$$\xi < \frac{\lambda}{8\pi r_0 Z}\left(\frac{I_p}{c^2}\right)^2, \tag{39}$$

where λ is the laser wavelength and r_0 is the classical radius of the electron. We can see that in the relativistic regime it is possible to realize the tunneling ionization with $\gamma \ll 1$ when the discrepancy between the gauge-invariant SFA and the

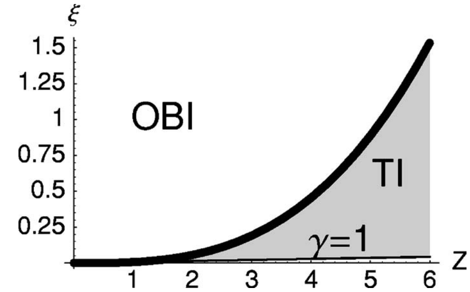

FIG. 1. The region of parameters ξ and Z where different ionization regimes of a hydrogenlike ion take place. The thin curve at the bottom corresponds the condition of $\gamma=1$. The tunneling ionization (TI) regime takes place for the parameters of the shaded region [see Eqs. (38) and (39)], and the over-the-barrier ionization (OBI) for the parameters above the thick curve.

conventional SFA with the velocity gauge is large.

To evaluate the difference of predictions of the ionization probability by these two versions of the SFA more precisely, we have carried out numerical calculations of the direct ionization amplitude of Eq. (36) applying the saddle point method. The atomic potential in Eq. (36) is approximated by the Lewenstein short-range potential [9] with its matrix elements

$$\langle \mathbf{p}|V|0\rangle = \frac{\kappa^{3/2}}{2\pi p}, \quad V_{\mathbf{p},\mathbf{q}} = \frac{\kappa}{4\pi^2 pq}. \tag{40}$$

In Fig. 2 we compare the ionization probability calculated by means of the gauge-invariant SFA of Eq. (36) with the result of the conventional SFA in the velocity gauge [i.e., the amplitude of Eq. (35) where as an initial state a free-atomic wave function is used]. We see that the difference can be significant, the ratio of the amplitudes reaching two orders of magnitude.

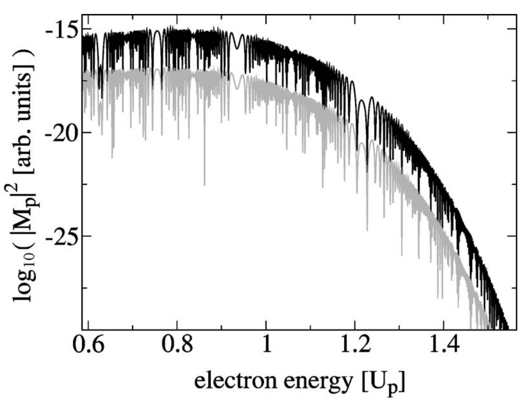

FIG. 2. Photoelectron spectrum in a linearly polarized laser field with angular frequency $\omega=0.05$ a.u. and electric field strength $E=3.4$ a.u. via $\log_{10}(|M_{\mathbf{p}}|^2)$ in Eq. (36), with final electron momentum $\mathbf{p}=(p_x,0,p_z)$ and emission angle $\theta=\arccos(p_x/p)=0.18$. The model potential is adapted to B^{4+} with ionization potential $I_p=12.5$ a.u. The electron energy is scaled in multiples of the ponderomotive energy $U_p=\langle A^2/2\rangle$. The photoelectron spectrum in gray is evaluated via the standard SFA in the velocity gauge, the one in black via the gauge-invariant SFA.

III. THE DIRAC REGIME

In this section we generalize the gauge-invariant SFA for the relativistic regime based on the Dirac equation

$$i\partial_t\Psi = [c\boldsymbol{\alpha}\cdot(\mathbf{p}+\mathbf{A}/c) - \phi + V + \beta c^2]\Psi, \tag{41}$$

where $\boldsymbol{\alpha}$ and β are the corresponding Dirac-matrices.

Analogous to the Schrödinger and the Klein-Gordon cases, we employ the ansatz of Eq. (7) with the Floquet eigenstates of the total Hamiltonian $\Psi_n(x)=\exp(-i\varepsilon_n t)\Phi_n(x)$, the quasienergy ε_n, and the periodic quasienergy states $\Phi_n(x)$, yielding

$$i\partial_t\Psi_n = [c\boldsymbol{\alpha}\cdot(\mathbf{p}+\mathbf{A}/c) - \phi + V + \beta c^2]\Psi_n. \tag{42}$$

The initial state $\Psi_0(x)=\exp(-i\varepsilon_0 t)\Phi_0(x)$ with the energy ε_0 is an eigenstate of the physical energy operator:

$$[c\boldsymbol{\alpha}\cdot(\mathbf{p}+\mathbf{A}/c) + V + \beta c^2]\Phi_0 = \varepsilon_0\Phi_0. \tag{43}$$

Using the orthonormality of the Floquet eigenstates $\langle\Phi_n|\Phi_k\rangle=\delta_{nk}$, we receive the following expression for the coefficients $c_n(t)$:

$$c_n = i\int_{-\infty}^{t} dt \int d\mathbf{r}\, \Psi_n^\dagger(x)[(\phi + i\partial_t)\Phi_0(x)]\exp\left(-i\int \varepsilon_0 dt\right). \tag{44}$$

In the SFA the exact eigenstate of the total Hamiltonian $\Psi_n(x)$ is replaced by the eigenstate of the electron in the laser field, i.e., by the relativistic Volkov wave function $\Psi_{\mathbf{p}}^V(x)$ [1],

$$i\partial_t\Psi_{\mathbf{p}}^V(x) = [c\boldsymbol{\alpha}\cdot(\mathbf{p}+\mathbf{A}/c) - \phi + \beta c^2]\Psi_{\mathbf{p}}^V(x). \tag{45}$$

We obtain for the amplitude of ionization in the relativistic regime

$$M_{\mathbf{p}} = -i\int d^4x\, \Psi_{\mathbf{p}}^{V\dagger}(x)[(\phi + i\partial_t)\Phi_0(x)]\exp\left(-i\int \varepsilon_0 dt\right). \tag{46}$$

The explicit expression for the amplitude (46) can be derived when we employ the initial-state wave function. In the Göppert-Mayer gauge, it obeys the quadratic Dirac equation

$$\left[\frac{[\varepsilon_0 - V]^2}{c^2} - \left(\hat{\mathbf{p}} - \frac{\mathbf{k}}{\omega}(\mathbf{E}\cdot\mathbf{r})\right)^2 - c^2 - \boldsymbol{\Sigma}\cdot\mathbf{H} + i\boldsymbol{\alpha}\cdot\mathbf{E}\right]\tilde{\Phi}_0(x) = 0, \tag{47}$$

where $\boldsymbol{\Sigma}$ is the spin matrix [18] and $\mathbf{E}$ and $\mathbf{H}$ the laser electric and magnetic fields, respectively. Equation (47) differs from the corresponding Klein-Gordon equation (30) by the last two terms of the spin interaction. The spin terms can be estimated by $\xi\omega$. Consequently, the ratio of the spin term to the p^2 one gives $\xi\omega/c^2$ and the spin terms can be neglected along with the other terms proportional to the laser field [see Eq. (31)]. As a result, the wave function for the initial state in the Göppert-Mayer gauge can be approximated by the four-spinor of the ground state of a free atom $\Phi_0(x)$. Inserting the latter in Eq. (46), we derive for the amplitude

$$M_{\mathbf{p}} = -i\int d^4x\, \Psi_{\mathbf{p}}^{V\dagger}(x)(\mathbf{E}\cdot\mathbf{r})\Psi_0(x). \tag{48}$$

We may derive another expression for the amplitude by applying partial time integration in Eq. (46) and using also Eq. (45),

$$M_{\mathbf{p}} = -i \int d^4x \, \Psi_{\mathbf{p}}^{V\dagger}(x) V \Psi_0(x). \qquad (49)$$

Thus, Eqs. (48) and (49) provide a gauge-invariant description of the ionization process in the fully relativistic regime within the SFA approach.

CONCLUSION

We have analyzed the choice of gauge in the relativistic SFA. The requirement to have a relativistic amplitude consistent with the conventional nonrelativistic SFA amplitude in the length gauge stipulates the use of the Göppert-Meyer gauge in the conventional relativistic SFA amplitude. To be able to use any gauge in the relativistic SFA, we have modified the standard SFA and obtained a gauge-invariant version of the relativistic SFA employing the eigenstate of the physical energy operator for the unperturbed bound state of the atomic system during the interaction. A comparison of the gauge-invariant SFA with the standard SFA in the radiation gauge, based on the numerical evaluation of the corresponding amplitudes, shows that the difference of the results can be significant, at some parameters in the relativistic regime approaching two orders of magnitude. Meanwhile in the nonrelativistic and weakly relativistic regimes the difference is not substantial. The nonrelativistic limit of the obtained amplitude of ionization coincides with the well-accepted conventional SFA amplitude in the length gauge.

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