Gauge-equivalent intense-field approximations in velocity and length gauges to all orders

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(Received 2 March 2007; published 14 June 2007)

A gauge invariant formulation of the so-called intense-field Keldysh-Faisal-Reiss (KFR) approximations in the "velocity" and "length" gauges is given and their equivalence is demonstrated term by term to *all* orders of the theory. It overcomes a long standing discrepancy between the velocity and the length gauge strong-field KFR amplitudes for nonperturbative processes in intense laser fields.

DOI: 10.1103/PhysRevA.75.063412 PACS number(s): 32.80.Rm, 32.80.Fb, 34.50.Fa, 42.50.Hz

I. INTRODUCTION

Investigations of atomic, molecular, and optical processes in intense laser fields are currently being pursued most vigorously. The so-called strong-field Keldysh-Faisal-Reiss (KFR) approximations [1–3] have provided fruitful insights into a wide range of highly nonperturbative processes in intense fields (e.g., [4]). However, the strong-field approximations in the "velocity" and "length" gauges differ and apparently constitute two distinct models. In the last several decades many authors have discussed the problem of gauge invariance of the KFR approximations, and various arguments have been advanced to justify the use of one or the other approximation in practice. In this paper we derive explicit expressions of the strong-field transition amplitudes in the velocity and length gauges and demonstrate their equivalence, term by term, in all orders, exactly. It provides an infinite series representation of the gauge-invariant KFR transition amplitude [cf [8]].

II. QUANTUM MECHANICAL GAUGE TRANSFORMATION

A. Form invariance

According to the minimal coupling scheme, the Schrödinger equation of an electron interacting with an electromagnetic field, is given by

$$\left(i\hbar\frac{\partial}{\partial t} - eA_0\right)|\Psi(t)\rangle = \frac{\left(\boldsymbol{p}_{op} - \frac{e}{c}\boldsymbol{A}\right)^2}{2m}|\Psi(t)\rangle, \tag{1}$$

where $A_0 \equiv A_0(\mathbf{r},t)$ is the scalar and $\boldsymbol{A} \equiv \boldsymbol{A}(\boldsymbol{r},t)$ is the vector potential. The quantum mechanical gauge transformation consists in changing the potentials by a scalar function $\xi = \xi(\boldsymbol{r},t)$, which leaves the electromagnetic field strengths unchanged and simultaneously changing the wave function by the gauge factor $e^{-i(e/\hbar c)\xi}$,

$$A_0 \to \tilde{A}_0 = A_0 + \frac{1}{c}\frac{\partial \xi}{\partial t},$$

$$\boldsymbol{A} \to \tilde{\boldsymbol{A}} = \boldsymbol{A} - \frac{\partial \xi}{\partial \boldsymbol{r}},$$

$$|\Psi(t)\rangle \to |\tilde{\Psi}(t)\rangle = e^{-i(e/\hbar c)\xi}|\Psi(t)\rangle. \tag{2}$$

Substituting Eq. (2) in Eq. (1) and performing the simple calculations, one obtains in the new gauge

$$\left(i\hbar\frac{\partial}{\partial t} - e\tilde{A}_0\right)|\tilde{\Psi}(t)\rangle = \frac{\left(\boldsymbol{p}_{op} - \frac{e}{c}\tilde{\boldsymbol{A}}\right)^2}{2m}|\tilde{\Psi}(t)\rangle. \tag{3}$$

Thus, the essence of the gauge transformation in quantum mechanics is the invariance of the form of the Schrödinger equation with respect to the potentials in the old and in the new (tilde) gauges, as it is immediately apparent from the form of Eqs. (1) and (3). This ensures the requirement of physical invariance of the transition probabilities (and the expectation values of Hermitian observables) in the old and the new gauges. Furthermore, the gauge invariance of the (transition) probabilities implies that the transition amplitudes must also be the same to with in a constant phase factor, in the two gauges.

B. Total Hamiltonians: Velocity gauge and length gauge

The minimal coupling Schrödinger equation (1) in the dipole approximation (when $\boldsymbol{A}(t)$ becomes a function of t only) defines the total Hamiltonian $H(t)$ in the so-called velocity gauge

$$H(t) = \frac{\left[\boldsymbol{p}_{op} - \frac{e}{c}\boldsymbol{A}(t)\right]^2}{2m} + V \text{ (velocity gauge)}, \tag{4}$$

where we have set $eA_0 \equiv V$ for the binding potential. Using the gauge function in the dipole approximation $\xi(\boldsymbol{r},t) = \boldsymbol{A}(t)\cdot\boldsymbol{r}$, and the gauge transformation equations (2), one immediately calculates

$$\tilde{A}_0 = A_0 + \frac{1}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r},$$

$$\tilde{\boldsymbol{A}} = \boldsymbol{A} - \boldsymbol{A},$$

$$= 0. \tag{5}$$

Thus, from Eq. (3), we get the total Hamiltonian in the new (the so-called length) gauge

$$\tilde{H}(t) = \frac{\boldsymbol{p}_{op}^2}{2m} + V + \frac{e}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r},$$

$$= \frac{\boldsymbol{p}_{op}^2}{2m} + V - e\boldsymbol{E}(t)\cdot\boldsymbol{r} \text{ (length gauge)}, \tag{6}$$

where we have used the definition $\boldsymbol{E}(t) = -\frac{1}{c}\dot{\boldsymbol{A}}(t)$.

III. TIME-DEPENDENT GREEN'S FUNCTION AND TRANSITION AMPLITUDE

A. Time-dependent Green's function

Let the Schrödinger equation of the interacting system with a total Hamiltonian $H(t)$ be

$$\left[i\hbar\frac{\partial}{\partial t} - H(t)\right]|\Psi(t)\rangle = 0. \tag{7}$$

We define the Green's function (or propagator) $G(t,t_0)$ associated with $H(t)$, by the inhomogeneous equation

$$\left[i\hbar\frac{\partial}{\partial t} - H(t)\right]G(t,t_0) = \delta(t-t_0). \tag{8}$$

The solution of the Schrödinger equation (7) which satisfies the general initial condition

$$|\Psi(t)\rangle = 0, \quad t < t_0,$$

$$|\Psi(t)\rangle = |\phi_i(t_0)\rangle, \quad t = t_0^{(+)}, \tag{9}$$

where $|\phi_i(t_0)\rangle$ is the initial state of the system prepared at $t = t_0$, is given by

$$|\Psi(t)\rangle = i\hbar G(t,t_0)|\phi_i(t_0)\rangle. \tag{10}$$

The solution (10) of Eq. (7) is readily verified by operating on Eq. (10) with $[i\hbar\frac{\partial}{\partial t} - H(t)]$, using Eq. (8), and noting that due to the resulting delta function, Eq. (7) is fulfilled for all t not equal to t_0. For $t=t_0$, an integration in the immediate neighborhood of the singularity reproduces the initial condition (9).

We use a convenient expression of the total propagator G of the system, in terms of the partial propagators G_0 and G_f associated with the partial Hamiltonians H_0 and H_f, defined by the two partitions of the total Hamiltonian $H(t)=H_0(t) + V_0(t)$ and $H(t)=H_f(t)+V_f(t)$, respectively. Then for any t between the initial-time t_0 and the final-time t_f, we have a convenient series expansion of $G(t,t_0)$ in the form (see Refs. [4] or [5]),

$$G(t,t_0) = G_0(t,t_0) + \int_{t_0}^{t_f} dt_1 G_f(t,t_1)V_0(t_1)G_0(t_1,t_0) + \int_{t_0}^{t_f}\int_{t_0}^{t_f} dt_2 dt_1 G_f(t,t_2)V_f(t_2)G_f(t_2,t_1)V_0(t_1)G_0 \times(t_1,t_0) + \cdots . \tag{11}$$

B. "Prior series" of transition amplitude

The probability amplitude of a transition from a (noninteracting) initial state $|\phi_i(t_0)\rangle$, prepared at $t=t_0$, to a final state $|\Phi_f(t_f)\rangle$ at $t=t_f$, is given by

$$S_{if} = \langle\Phi_f(t_f)|\Psi(t_f)\rangle = i\hbar\langle\Phi_f(t_f)|G(t_f,t_0)|\phi_i(t_0)\rangle, \tag{12}$$

where in the second line we have used Eq. (10). To obtain a systematic expansion of transition amplitudes of interest, we substitute Eq. (11) for $G(t,t_0)$ in Eq. (12), and obtain the "*prior* series" (see [4,5]) for the transition amplitude between the initial state $|\phi_i(t_0)\rangle$ and the final state $|\Phi_f(t_f)\rangle$ to any desired order:

$$S_{if} = \sum_{n=0}^{\infty} S_{if}^{(n)} \tag{13}$$

with

$$S_{if}^{(0)} = i\hbar\langle\Phi_f(t_f)|G_0(t_f,t_0)|\phi_i(t_0)\rangle \tag{14}$$

$$S_{if}^{(1)} = i\hbar\int dt_1\langle\Phi_f(t_f)|G_f(t_f,t_1)V_0(t_1)G_0(t_1,t_0)|\phi_i(t_0)\rangle \tag{15}$$

$$S_{if}^{(2)} = i\hbar\int dt_2 dt_1\langle\Phi_f(t_f) \times|G_f(t_f,t_2)V_f(t_2)G_f(t_2,t_1)V_0(t_1)G_0(t_1,t_0)|\phi_i(t_0)\rangle \tag{16}$$

$$\cdots = \cdots$$

$$S_{if}^{(n)} = i\hbar\int dt_n dt_{n-1}\cdots dt_2 dt_1\langle\Phi_f(t_f)|G_f(t_f,t_n)V_f(t_n) \times G_f(t_n,t_{n-1})V_f(t_{n-1})\cdots G_f(t_2,t_1)V_0(t_1) \times G_0(t_1,t_0)|\phi_i(t_0)\rangle, \tag{17}$$

where $\int$ stands for the (multiple) integrations in the same range t_0 to t_f. For the sake of simplicity, in the sequel we shall assume the usual dipole (or long-wavelength) approximation in which the vector potential $\boldsymbol{A}(t)$ and the electric field strength $\boldsymbol{E}(t) \equiv -\frac{1}{c}\dot{\boldsymbol{A}}(t)$ become functions of t only. The gauge function, ξ, can be chosen explicitly to be $\xi(\boldsymbol{r},t) = \boldsymbol{A}(t)\cdot\boldsymbol{r}$.

C. Field-free conditions

For a dynamic transition process, it is important to ensure the initial and the final conditions, including that of the laser pulse, to define the unique physical transition process in the laboratory, in both the gauges unambiguously. We assume as usual that, in the laboratory, the initial state is "prepared" at t_0 before the interaction, and the final state is "observed" at t_f after the interaction with the laser pulse, e.g.,

$$\boldsymbol{A}(t_0) = 0. \tag{18}$$

IV. TRANSITION AMPLITUDE IN VELOCITY GAUGE

A. Initial-state partition

We partition the total Hamiltonian (4), as usual, as $H(t) = H_0(t) + V_0(t)$, where

$$H_0(t) = \frac{\boldsymbol{p}_{op}^2}{2m} + V \tag{19}$$

and

$$V_0(t) = -\frac{e}{mc}\boldsymbol{A}(t)\cdot\boldsymbol{p}_{op} + \frac{e^2}{2mc^2}A^2(t). \tag{20}$$

The exact solutions of interest of Eq. (19) are

$$|\phi_j(t)\rangle = e^{-(i/\hbar)H_a t}|\phi_j\rangle, \tag{21}$$

where $|\phi_j\rangle$ form a complete set of orthonormal eigenfunctions of the "atomic" Schrödinger equation

$$H_a|\phi_j\rangle = \left(\frac{\boldsymbol{p}_{op}^2}{2m} + V\right)|\phi_j\rangle = E_j|\phi_j\rangle, \tag{22}$$

for all index j (discrete and continuous). They satisfy the orthonormal condition

$$\langle\phi_{j'}(t)|\phi_j(t)\rangle = \delta_{j',j}, \tag{23}$$

and form a complete set

$$\sum_j |\phi_j(t)\rangle\langle\phi_j(t)| = \mathbf{1}. \tag{24}$$

Thus, the propagator $G_0(t,t_0)$ associated with $H_0(t)$, that satisfies an equation analogous to Eq. (8) with $H(t)$ replaced by $H_0(t)$ (similar equations hold for the other propagators defined below), can be easily written down,

$$G_0(t,t_0) = -\frac{i}{\hbar}\theta(t-t_0)\sum_j |\phi_j(t)\rangle\langle\phi_j(t_0)|, \tag{25}$$

where the symbol Σ_j stands both for the sum over the discrete and the integration over the continuous indices.

B. Final-state partition

Next, we introduce the final-state partition $H(t) = H_f(t) + V_f(t)$, where

$$H_f(t) = \frac{\left[\boldsymbol{p}_{op} - \frac{e}{c}\boldsymbol{A}(t)\right]^2}{2m}, \tag{26}$$

$$V_f(t) = V. \tag{27}$$

The final reference propagator $G_f(t,t')$ associated with the Hamiltonian (26) can be written in terms of the complete set of the well-known Volkov wave functions in the velocity gauge (e.g., [6]),

$$|\Phi_{\boldsymbol{p}}(t)\rangle = L^{-3/2}|\boldsymbol{p}\rangle\exp\left(-\frac{i}{\hbar}\int^t \frac{\left[\boldsymbol{p} - \frac{e}{c}\boldsymbol{A}(t')\right]^2}{2m}dt'\right), \tag{28}$$

where L^3 is the normalization volume, lim $L\to\infty$; $|\boldsymbol{p}\rangle$ is a plane-wave of momentum $\boldsymbol{p}$: $\langle\boldsymbol{r}|\boldsymbol{p}\rangle = e^{(i/\hbar)\boldsymbol{p}\cdot\boldsymbol{r}}$. The Volkov states satisfy the orthogonality condition

$$\langle\Phi_{\boldsymbol{p}'}(t)|\Phi_{\boldsymbol{p}}(t)\rangle = \delta_{\boldsymbol{p}'\boldsymbol{p}} \tag{29}$$

and the completeness relation

$$\sum_{\boldsymbol{p}} |\Phi_{\boldsymbol{p}}(t)\rangle\langle\Phi_{\boldsymbol{p}}(t)| = \mathbf{1}. \tag{30}$$

Hence, the Volkov propagator in the velocity gauge can be written as

$$G_f(t,t') = -\frac{i}{\hbar}\theta(t-t')\sum_{\boldsymbol{p}} |\Phi_{\boldsymbol{p}}(t)\rangle\langle\Phi_{\boldsymbol{p}}(t')|. \tag{31}$$

C. All order amplitudes: Velocity gauge

To obtain the intense-field transition amplitudes in the velocity gauge, we need only to substitute the explicit expressions of V_0, G_0, V_f, and G_f, given by Eqs. (20), (25), (27), and (31), respectively, in the general S-matrix terms, Eqs. (14)–(17), and simplify the algebra. To this end, first, we note the effect of operating with $G_0(t_1,t_0)$ on the initial state $|\phi_i(t_0)\rangle \equiv e^{-(i/\hbar)E_i t_0}|\phi_i\rangle$:

$$\begin{aligned} i\hbar G_0(t_1,t_0)|\phi_i(t_0)\rangle &= \theta(t_1-t_0)\sum_j |\phi_j(t_1)\rangle\langle\phi_j(t_0)|\phi_i(t_0)\rangle \\ &= |\phi_i(t_1)\rangle, \quad t_1 > t_0, \end{aligned} \tag{32}$$

where, we have used Eq. (21), and noted that $\langle\phi_j|\phi_i\rangle = \delta_{ij}$. Next, from the equal-time orthonormality of the Volkov states, Eq. (29), and the Volkov propagator, Eq. (31), we get

$$\langle\Phi_{\boldsymbol{p}_f}(t_f)|G_f(t_f,t)| = -\frac{i}{\hbar}\theta(t_f-t)\langle\Phi_{\boldsymbol{p}_f}(t)| = -\frac{i}{\hbar}\langle\Phi_{\boldsymbol{p}_f}(t)|, \quad t < t_f. \tag{33}$$

Thus, using Eqs. (32) and (18), for the zeroth order amplitude [see Eq. (14)] we find

$$S_{if}^{(0)} = i\hbar\langle\Phi_{\boldsymbol{p}_f}(t_f)|G_0(t_f,t_0)|\phi_i(t_0)\rangle = \langle\Phi_{\boldsymbol{p}_f}(t_f)|\phi_i(t_f)\rangle. \tag{34}$$

In a similar way, using Eqs. (32), (33), (20), and (18), we find for the first order amplitude [Eq. (15)]

$$S_{if}^{(1)} = \int_{t_0}^{t_f} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_1)|V_0(t_1)G_0(t_1,t_0)|\phi_i(t_0)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t_f} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_1)|V_0(t_1)|\phi_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t_f} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_1)|$$
$$\times\left(-\frac{e}{mc}\boldsymbol{A}(t_1)\cdot\boldsymbol{p}_{op} + \frac{e^2}{2mc^2}\boldsymbol{A}^2(t_1)\right)|\phi_i(t_1)\rangle, \quad (35)$$

where in the last line we have used Eq. (20) for $V_0(t)$. We may note, parenthetically, that the above amplitude corresponds to the "prior form" of the well-known KFR amplitude in the velocity gauge [2,3].

Proceeding in a similar way as above, for the second order amplitude [see Eq. (16)] we get

$$S_{if}^{(2)} = \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t_f}\int_{t_0}^{t_f} dt_2 dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_2)|VG_f(t_2,t_1)V_0(t_1)|\phi_i(t)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t_f}\int_{t_0}^{t_f} dt_2 dt_1 \theta(t_2-t_1)\sum_{\boldsymbol{p}} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}}(t_2)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}}(t_1)|V_0(t_1)|\phi_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2\int_{t_0}^{t_f} dt_2 \int_{t_0}^{t_2} dt_1 \sum_{\boldsymbol{p}} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}}(t_2)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}}(t_1)|\left(-\frac{e}{mc}\dot{\boldsymbol{A}}(t_1)\cdot\boldsymbol{p}_{op} + \frac{e^2}{2mc^2}\boldsymbol{A}^2(t_1)\right)|\phi_i(t_1)\rangle. \quad (36)$$

Continuing in an analogous manner, for the nth order amplitude in the velocity gauge [see Eq. (17)] we get the general result

$$S_{if}^{(n)} = \int dt_n dt_{n-1}\cdots dt_2 dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_n)|G_f(t_n,t_{n-1})$$
$$\times V\cdots G_f(t_2,t_1)V_0(t_1)|\phi_i(t)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^n \sum_{\boldsymbol{p}_{n-1},\ldots,\boldsymbol{p}_1}\int_{t_0}^{t_f} dt_n \int_{t_0}^{t_n} dt_{n-1}\cdots\int_{t_0}^{t_3} dt_2 \int_{t_0}^{t_2} dt_1$$
$$\times\langle \Phi_{\boldsymbol{p}_f}(t_n)|V|\Phi_{\boldsymbol{p}_{n-1}}(t_n)\rangle \times \langle \Phi_{\boldsymbol{p}_{n-1}}(t_{n-1})|V\cdots|\Phi_{\boldsymbol{p}_1}(t_2)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}_1}(t_1)|\left(-\frac{e}{mc}\dot{\boldsymbol{A}}(t_1)\cdot\boldsymbol{p}_{op} + \frac{e^2}{2mc^2}\boldsymbol{A}^2(t_1)\right)|\phi_i(t_1)\rangle. \quad (37)$$

V. TRANSITION AMPLITUDE IN LENGTH GAUGE

A. Initial-state partition

We rewrite the total Hamiltonian $\widetilde{H}(t)$ in the length gauge [Eq. (6)] by the addition of *zero*, i.e., by adding and subtracting a term

$$\widetilde{V}_0(t) = -\left[\frac{e}{mc}\boldsymbol{A}(t)\cdot\boldsymbol{p}_{op} + \frac{e^2}{2mc^2}A^2(t)\right] \quad (38)$$

as

$$\widetilde{H}(t) = \frac{\boldsymbol{p}_{op}^2}{2m} + V + \frac{e}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r} + [-\widetilde{V}_0(t) + \widetilde{V}_0(t)]$$
$$= \left(\frac{\left[\boldsymbol{p}_{op} + \frac{e}{c}\boldsymbol{A}(t)\right]^2}{2m} + V + \frac{e}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r}\right) + \widetilde{V}_0(t)$$
$$= \widetilde{H}_0(t) + \widetilde{V}_0(t), \quad (39)$$

where the reference Hamiltonian is now given by

$$\widetilde{H}_0(t) = \frac{\left[\boldsymbol{p}_{op} + \frac{e}{c}\boldsymbol{A}(t)\right]^2}{2m} + V + \frac{e}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r} \quad (40)$$

and the interaction Hamiltonian by $\widetilde{V}_0(t)$ above.

We consider the solution of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\widetilde{\psi}_j(t)\rangle = \widetilde{H}_0(t)|\widetilde{\psi}_j(t)\rangle, \quad (41)$$

where $\widetilde{H}_0(t)$ is defined by Eq. (40). The exact solutions of interest are

$$|\widetilde{\psi}_j(t)\rangle = e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}e^{-(i/\hbar)H_a t}|\phi_j\rangle, \quad (42)$$

where, $|\phi_j\rangle$ form a complete set of orthonormal eigenfunctions of the "atomic" Schrödinger Eq. (22). The validity of our solutions (42), can be readily verified by direct substitution in Eq. (41), and simplifying the algebra using

$$\left[\boldsymbol{p}_{op} + \frac{e}{c}\boldsymbol{A}(t)\right]|\widetilde{\psi}_j(t)\rangle = \left[\boldsymbol{p}_{op} + \frac{e}{c}\boldsymbol{A}(t)\right](e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}})|\phi_j(t)\rangle$$
$$= (e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}})(\boldsymbol{p}_{op})|\phi_j(t)\rangle, \quad (43)$$

where $|\phi_j(t)\rangle = e^{-(i/\hbar)H_a t}|\phi_j\rangle = e^{-(i/\hbar)E_j t}|\phi_j\rangle$. Note that the $|\widetilde{\psi}_j(t)\rangle$ are associated one-to-one with the $|\phi_j\rangle$, and thus they too satisfy the orthonormal condition

$$\langle\widetilde{\psi}_{j'}(t)|\widetilde{\psi}_j(t)\rangle = \delta_{j',j}, \quad (44)$$

and form a complete set

$$\sum_j |\widetilde{\psi}_j(t)\rangle\langle\widetilde{\psi}_j(t)| = \mathbf{1}, \quad (45)$$

where j runs over all discrete and continuous indices. Hence, the propagator $\widetilde{G}_0(t,t_0)$ associated with $\widetilde{H}_0(t)$, that satisfies an equation analogous to Eq. (8) with $H(t)$ replaced by $\widetilde{H}_0(t)$, can be easily written down as

$$\widetilde{G}_0(t,t_0) = -\frac{i}{\hbar}\theta(t-t_0)\sum_j |\widetilde{\psi}_j(t)\rangle\langle\widetilde{\psi}_j(t_0)|. \quad (46)$$

B. Final-state partition

Next, we introduce the final-state partition $\tilde{H}(t)=\tilde{H}_f(t)+\tilde{V}_f(t)$, where

$$\tilde{H}_f(t)=\frac{\boldsymbol{p}^2}{2m}+\frac{e}{c}\dot{\boldsymbol{A}}(t)\cdot\boldsymbol{r} \tag{47}$$

and

$$\tilde{V}_f(t)=V. \tag{48}$$

The well-known Volkov solutions in the length gauge (e.g., [6]), associated with $\tilde{H}_f(t)$, are

$$\begin{aligned}|\tilde{\Phi}_{\boldsymbol{p}}(t)\rangle &= L^{-3/2}\left|\left[\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}(t)\right]\right\rangle\\ &\quad\times\exp\left(-\frac{i}{\hbar}\int^t\frac{\left[\boldsymbol{p}-\frac{e}{c}\boldsymbol{A}(t')\right]^2}{2m}dt'\right)\\ &= e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}|\Phi_{\boldsymbol{p}}(t)\rangle,\end{aligned} \tag{49}$$

where $|\Phi_{\boldsymbol{p}}(t)\rangle$ is the Volkov solution in the velocity gauge (28). Therefore, the Volkov propagator in the length gauge $\tilde{G}_f(t,t')$ can be written in terms of the Volkov propagator in the velocity gauge $G_f(t,t')$, Eq. (31):

$$\begin{aligned}\tilde{G}_f(t,t') &= -\frac{i}{\hbar}\theta(t-t')|\tilde{\Phi}_{\boldsymbol{p}}(t)\rangle\langle\tilde{\Phi}_{\boldsymbol{p}}(t')|,\\ &= e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}G_f(t,t')e^{+i(e/\hbar c)\boldsymbol{A}(t')\cdot\boldsymbol{r}}.\end{aligned} \tag{50}$$

C. All order amplitudes: Length gauge

To obtain the transition amplitudes in successive orders in the present case, we need simply to substitute the tilde quantities (length gauge) $\tilde{G}_0$, $\tilde{V}_0$, $\tilde{G}_f$, and $\tilde{V}_f$, defined above, in place of the respective nontilde quantities, in the formal expressions for the amplitudes (14)–(17), and simplify the algebra. To this end, first, we note the effect of operating with $\tilde{G}_0(t_1,t_0)$ on the initial state $|\tilde{\phi}_i(t_0)\rangle=|\phi_i(t_0)\rangle=e^{-(i/\hbar)E_it_0}|\phi_i\rangle$:

$$\begin{aligned}i\hbar\tilde{G}_0(t_1,t_0)|\tilde{\phi}_i(t_0)\rangle &= \theta(t_1-t_0)\sum_j|\tilde{\psi}_j(t_1)\rangle\langle\tilde{\psi}_j(t_0)|\tilde{\phi}_i(t_0)\rangle\\ &= \theta(t_1-t_0)\sum_j|\tilde{\psi}_j(t_1)\rangle\delta_{ij}\\ &= |\tilde{\psi}_i(t_1)\rangle,\quad t_1>t_0.\end{aligned} \tag{51}$$

In the second line above we have used Eq. (18) and noted that $\langle\phi_j|\phi_i\rangle=\delta_{ij}$.

Next, from the equal-time orthonormality of the Volkov states (49) and the Volkov propagator (50) we get

$$\begin{aligned}\langle\tilde{\Phi}_{\boldsymbol{p}_f}(t_f)|\tilde{G}_f(t_f,t)| &= -\frac{i}{\hbar}\theta(t_f-t)\langle\tilde{\Phi}_{\boldsymbol{p}_f}(t)|\\ &= -\frac{i}{\hbar}\langle\Phi_{\boldsymbol{p}_f}(t)|(e^{+i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}),\quad t<t_f.\end{aligned} \tag{52}$$

Thus, using Eqs. (51) and (49), we find for the zeroth order amplitude [see Eq. (14)]

$$\tilde{S}_{if}^{(0)}=i\hbar\langle\tilde{\Phi}_{\boldsymbol{p}_f}(t_f)|\tilde{G}_0(t_f,t_0)|\tilde{\phi}_i(t_0)\rangle=\langle\Phi_{\boldsymbol{p}_f}(t_f)|\phi_i(t_f)\rangle=S_{if}^{(0)}, \tag{53}$$

where; the last equality follows from a comparison with Eq. (34).

Similarly, from the definition of the first order amplitude (15) we get

$$\begin{aligned}\tilde{S}_{if}^{(1)} &= \int_{t_0}^{t_f}dt_1\langle\tilde{\Phi}_{\boldsymbol{p}_f}(t_1)|\tilde{V}_0(t_1)\tilde{G}_0(t_1,t_0)|\tilde{\phi}_i(t_0)\rangle\\ &= \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t_f}dt_1\langle\Phi_{\boldsymbol{p}_f}(t_1)|e^{i(e/\hbar c)\boldsymbol{A}(t_1)\cdot\boldsymbol{r}}\tilde{V}_0(t_1)|\tilde{\psi}_i(t_1)\rangle\\ &= \left(-\frac{i}{\hbar}\right)\int_{t_0}^{t_f}dt_1\langle\Phi_{\boldsymbol{p}_f}(t_1)|\left[-\frac{e}{mc}\boldsymbol{A}(t_1)\cdot\boldsymbol{p}_{op}+\frac{e^2}{2mc^2}A^2(t_1)\right]\\ &\quad\times|\phi_i(t_1)\rangle=S_{if}^{(1)},\end{aligned} \tag{54}$$

where we have used the identity

$$\begin{aligned}&e^{i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}\tilde{V}_0(t)e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}\\ &\quad= e^{i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}\left\{-\left[\frac{e}{mc}\boldsymbol{A}(t)\cdot\boldsymbol{p}_{op}+\frac{e^2}{2mc^2}A^2(t)\right]\right\}\\ &\quad\times e^{-i(e/\hbar c)\boldsymbol{A}(t)\cdot\boldsymbol{r}}\\ &\quad= \left(-\frac{e}{mc}\boldsymbol{A}(t)\cdot\boldsymbol{p}_{op}+\frac{e^2}{2mc^2}A^2(t)\right)\\ &\quad= V_0(t).\end{aligned} \tag{55}$$

The last equality in Eq. (54) follows from a comparison with Eq. (35).

Next, we consider the higher order amplitudes in the length gauge. Using Eqs. (51) and (52) in the second order amplitude (16) and remembering that $\tilde{V}_f(t)=V$, we get

$$\tilde{S}_{if}^{(2)} = \left(-\frac{i}{\hbar}\right) \int dt_2 dt_1 \langle \tilde{\Phi}_{\boldsymbol{p}_f}(t_2)|\tilde{V}_f(t_2)\tilde{G}_f(t_2,t_1)\tilde{V}_0(t_1)|\tilde{\psi}_i(t)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t_f}\int_{t_0}^{t_f} dt_2 dt_1 \theta(t_2-t_1)\sum_{\boldsymbol{p}_1} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}_1}(t_2)\rangle \times \langle \Phi_{\boldsymbol{p}_1}(t_1)|e^{i(e/\hbar c)\boldsymbol{A}(t_1)\cdot \boldsymbol{r}}\tilde{V}_0(t_1)|\tilde{\psi}_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t_f} dt_2 \int_{t_0}^{t_2} dt_1 \sum_{\boldsymbol{p}_1} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}_1}(t_2)\rangle \times \langle \Phi_{\boldsymbol{p}_1}(t_1)|e^{i(e/\hbar c)\boldsymbol{A}(t_1)\cdot \boldsymbol{r}}\tilde{V}_0(t_1)e^{-i(e/\hbar c)\boldsymbol{A}(t_1)\cdot \boldsymbol{r}}|\phi_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t_f} dt_2 \int_{t_0}^{t_2} dt_1 \sum_{\boldsymbol{p}_1} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}_1}(t_2)\rangle \times \langle \Phi_{\boldsymbol{p}_1}(t_1)|V_0(t_1)|\phi_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t_f} dt_2 \int_{t_0}^{t_2} dt_1 \sum_{\boldsymbol{p}_1} \langle \Phi_{\boldsymbol{p}_f}(t_2)|V|\Phi_{\boldsymbol{p}_1}(t_2)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}_1}(t_1)|\left[-\frac{e}{mc}\boldsymbol{A}(t)\cdot \boldsymbol{p}_{op} + \frac{e^2}{2mc^2}A^2(t_1)\right]|\phi_i(t_1)\rangle = S_{if}^{(2)}, \tag{56}$$

where we have used Eq. (42) and the identity (55) in the equations above and the last equality follows from a comparison with Eq. (36).

Continuing in an analogous way, and using Eqs. (51) and (52) in the nth order amplitude [Eq. (17)], we get, first,

$$\tilde{S}_{if}^{(n)} = \left(-\frac{i}{\hbar}\right) \int dt_n dt_{n-1} \cdots dt_2 dt_1 \langle \tilde{\Phi}_{\boldsymbol{p}_f}(t_n)|\tilde{V}_f(t_n)\tilde{G}_f(t_n,t_{n-1})$$
$$\times \tilde{V}_f(t_{n-1}) \cdots \tilde{G}_f(t_2,t_1)\tilde{V}_0(t_1)|\tilde{\psi}_i(t_1)\rangle. \tag{57}$$

This expression can be further reduced using successively the identity

$$\langle \tilde{\Phi}_{p_j}(t_j)|\tilde{V}_f(t_j)\tilde{G}_f(t_j,t_{j-1})$$
$$= -\frac{i}{\hbar}\theta(t_j-t_{j-1})\sum_{\boldsymbol{p}_{j-1}} \langle \Phi_{\boldsymbol{p}_j}(t_j)|V|\Phi_{\boldsymbol{p}_{j-1}}(t_j)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}_{j-1}}(t_{j-1})|(e^{i(e/\hbar c)\boldsymbol{A}(t_{j-1})\cdot \boldsymbol{r}}), \tag{58}$$

where $j=2,3,\ldots,n$ and $\boldsymbol{p}_n \equiv \boldsymbol{p}_f$, which is readily established from Eqs. (48)–(50). Thus, noting the presence of the theta functions (associated with the propagators) which determine the integration intervals, and applying the identity (58) to the nth order amplitude (57), we finally deduce,

$$\tilde{S}_{if}^{(n)} = \left(-\frac{i}{\hbar}\right)^n \sum_{\boldsymbol{p}_{n-1},\ldots,\boldsymbol{p}_1} \int_{t_0}^{t_f} dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_3} dt_2$$
$$\times \int_{t_0}^{t_2} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_n)|V|\Phi_{\boldsymbol{p}_{n-1}}(t_n)\rangle \times \langle \Phi_{\boldsymbol{p}_{n-1}}(t_{n-1})| \ldots$$
$$\times V|\Phi_{\boldsymbol{p}_1}(t_2)\rangle\langle \Phi_{\boldsymbol{p}_1}(t_1)|e^{i(e/\hbar c)\boldsymbol{A}(t_1)\cdot \boldsymbol{r}}\tilde{V}_0(t_1)|\tilde{\psi}_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^n \sum_{\boldsymbol{p}_{n-1},\ldots,\boldsymbol{p}_1} \int_{t_0}^{t_f} dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots$$
$$\times \int_{t_0}^{t_3} dt_2 \int_{t_0}^{t_2} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_n)|V|\Phi_{\boldsymbol{p}_{n-1}}(t_n)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}_{n-1}}(t_{n-1})|V \cdots |\Phi_{\boldsymbol{p}_1}(t_2)\rangle\langle \Phi_{\boldsymbol{p}_1}(t_1)|V_0(t_1)|\phi_i(t_1)\rangle$$
$$= \left(-\frac{i}{\hbar}\right)^n \sum_{\boldsymbol{p}_{n-1},\ldots,\boldsymbol{p}_1} \int_{t_0}^{t_f} dt_n \int_{t_0}^{t_n} dt_{n-1} \cdots \int_{t_0}^{t_3} dt_2$$
$$\times \int_{t_0}^{t_2} dt_1 \langle \Phi_{\boldsymbol{p}_f}(t_n)|V|\Phi_{\boldsymbol{p}_{n-1}}(t_n)\rangle$$
$$\times \langle \Phi_{\boldsymbol{p}_{n-1}}(t_{n-1})|V \cdots |\Phi_{\boldsymbol{p}_1}(t_2)\rangle\langle \Phi_{\boldsymbol{p}_1}(t_1)|$$
$$\times \left(-\frac{e}{mc}\boldsymbol{A}(t_1)\cdot \boldsymbol{p}_{op} + \frac{e^2}{2mc^2}A^2(t)\right)|\phi_i(t_1)\rangle$$
$$= S_{if}^{(n)}. \tag{59}$$

The last equality, which follows from a comparison with Eq. (37), establishes the desired gauge invariance of the intense-field approximations, in the velocity and length gauges, in *all* orders, exactly.

VI. REMARKS AND SUMMARY

A. Remarks

Before concluding we observe the following.

(a) The gauge-equivalent KFR transition amplitude derived above is given by the infinite series representation, beginning with the leading terms (53) ($n=0$) and (54) ($n=1$), and followed by Eq. (59), for all successive terms ($n \geqslant 2$) of the series. Using an alternative partition of the total Hamiltonian one can obtain the gauge-invariant KFR amplitude in terms of an alternative infinite series [7], presented elsewhere [8]. At present little rigorous is known about the domains of convergence of the gauge-invariant KFR series. It is useful, however, to note that additional representations of the gauge-invariant amplitude may be constructed using a Shank's transformation [9], that could, in practice, provide a more rapid estimate of the series than their direct partial sums.

(b) For a long (or adiabatic) laser pulse, it is often convenient to Fourier transform the periodic part of the integrand with respect to t_n, in any order $n=1,2,3,\ldots$, and to carry out the final dt_n integration analytically between the limits $t_0 \to -\infty$ and $t_f \to \infty$, to obtain

$$S_{if}^{(n)} = -\frac{2\pi i}{L^{3/2}} \sum_s T_s^{(n)}(\boldsymbol{p}_f) \times \delta\left(\frac{p_f^2}{2m} + |E_i| + U_p - s\hbar\omega\right),$$
$$s = 0, \pm 1, \pm 2, \pm 3, \ldots \quad , \tag{60}$$

where $T_s^{(n)}(\boldsymbol{p}_f)$ is the sth Fourier component of the periodic part of the nth order amplitude. This allows one immediately to determine the bound-free transition probability per unit time, or the fundamental *rate* of the process, from the (generalized Fermi golden) rule

$$d\Gamma(\boldsymbol{p}_f) = \frac{2\pi}{\hbar} \sum_{s \geq s_0} \left| \sum_n T_s^{(n)}(\boldsymbol{p}_f) \right|^2 \times \delta\left(\frac{p_f^2}{2m} + |E_i| + U_p - s\hbar\omega\right) \frac{d^3 p_f}{(2\pi\hbar)^3}, \tag{61}$$

where $s_0 \equiv \left[\frac{(p_f^2/2m + |E_i| + U_p)}{\hbar\omega}\right]_{\text{int}} + 1$, $U_p \equiv \frac{e^2 F_0^2}{4m\omega^2}$ is the so-called ponderomotive energy, ω is the carrier frequency, and F_0 is the peak field strength.

(c) For an ultrashort laser pulse, when a steady rate of the transition $(i \to f, i \neq f)$ might be absent, one can simply take the absolute square of the sum of the time-dependent amplitudes (35)–(37) to obtain the transition probability of interest directly.

B. Summary

To summarize, a theory of intense-field transition amplitudes in "velocity" and "length" gauges is presented which explicitly demonstrates their equivalence, term by term, in all orders. Our results thus overcome an apparent long standing gauge discrepancy between the strong-field KFR amplitudes in the velocity and the length gauges.

ACKNOWLEDGMENTS

I would like to thank W. Mafezzoni-Faisal for a stimulating discussion and for her interest in the problem. This work was partially supported by the National Science Foundation through a grant for the Institute for Theoretical Atomic, Molecular and Optical Physics at Harvard University and Smithsonian Astrophysical Observatory.

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