

Acceleration-gauge Hamiltonian for a laser-driven particle with a position-dependent massMilan Šindelka^{✉,*}, Anael Ben-Asher,[†] and Nimrod Moiseyev[‡]*Institute of Plasma Physics, Academy of Sciences of the Czech Republic, Za Slovankou 1782/3, 18200 Prague 8, Czech Republic;**Schulich Faculty of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel;**and Faculty of Physics and Solid State Institute, Technion-Israel Institute of Technology, Haifa 32000, Israel*

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We address theoretically the problem of laser-induced dynamics of an electron, whose effective mass is position dependent (e.g., due to an effect of a semiconductor nanostructure environment). We derive the associated classical acceleration-gauge Hamiltonian $H_{AG}(t)$ under the most general conditions, even without imposing the dipole approximation. It is shown that $H_{AG}(t)$ possesses an intriguing structure arising due to the spatial dependence of the electronic mass. Subsequently, we restrict ourselves to a weak-field intensity regime, and derive the corresponding quantum mechanical acceleration-gauge Hamiltonian $\hat{H}_{AG}(t)$ which differs from its classical counterpart by an extra quantum term, \widehat{QM} . Our theoretical findings are illustrated numerically by calculating the probability $|T(E)|^2$ of the resonance transmission of an electron through a model semiconductor nanostructure. It is demonstrated that the quantum mechanical \widehat{QM} term of $\hat{H}_{AG}(t)$ does often affect crucially the profile of $|T(E)|^2$.

DOI: [10.1103/PhysRevA.103.053117](https://doi.org/10.1103/PhysRevA.103.053117)**I. INTRODUCTION**

The purpose of this work is to generalize the concept of the acceleration-gauge (AG) representation [1] to a situation when a charged particle with a *position-dependent mass* undergoes laser driving in the presence of an external potential. This study is partially motivated by our recent paper [2], where we have investigated the transmission of an electron through a semiconductor nanostructure in the presence of a weak monochromatic laser field. The theory presented in Ref. [2] was based upon the AG, and we have tacitly assumed that the effective (renormalized) mass of the electron moving in the semiconductor nanostructure environment is constant (i.e., position independent). However, in most if not all experimental arrangements involving semiconductor nanostructures, the renormalized electron mass actually does depend appreciably upon position [3,4], as the chemical composition of the semiconductor substrate is varied intentionally from layer to layer in order to create potential barriers or wells. This fact naturally prompts us to formulate the AG theory adequate for such circumstances.

For the case of a constant mass, the concept of AG representation was first introduced by Kramers and Henneberger [1]. Subsequently, the AG became well established as a valuable element of the toolset of theoretical atomic, molecular, and optical (AMO) physics. Indeed, the AG has proven its merits in enabling the physical interpretation of such phenomena as high-harmonic generation and above threshold ionization [5], the strong-field and high-frequency stabiliza-

tion effect [6], enhancement/suppression of tunneling by weak laser driving [7], laser-assisted scattering [2,8], and even in the context of forming unusual chemical bonds between atoms dressed by laser light [9], or for the creation of an artificial laser-generated atom with no nucleus [10]. The just mentioned examples strongly suggest that looking for the AG representation, for the case of a position-dependent mass, constitutes *per se* a legitimate and promising direction of research.

The structure of the paper is as follows. In Sec. II we give an overview of our most significant theoretical results and their numerical illustrations, while emphasizing the physical contents, and suppressing deliberately all the technical details regarding the underlying derivations and computations. On the other hand, Sec. III is devoted exclusively to a systematic self-contained technical elaboration and discussion of all the theory sketched in Sec. II. Those readers who wish to focus mainly on the physics phenomena may prefer to skip Sec. III in their first reading. Section IV describes then rather thoroughly our numerical calculations (and the underlying scattering theory of electrons through semiconductor nanostructures). Finally, Sec. V contains the concluding remarks.

II. OVERVIEW OF THE MAIN RESULTS**A. The general acceleration-gauge Hamiltonian**

We consider a charged nonrelativistic quantum particle (e.g., an electron) which is exposed to driving by an externally prescribed classical electromagnetic field $A(t, \mathbf{x})$ (e.g., by a laser pulse). The particle resides in a semiconductor nanostructure environment, which modifies its physical mass m into an effective position-dependent mass $m(\mathbf{x})$. An adequate momentum-gauge (MG) Hamiltonian describing the just

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introduced problem reads as follows [3]:

$$\hat{H}_{\text{MG}}(t) = \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(t, \hat{\mathbf{x}}) \right) \frac{1}{2m(\hat{\mathbf{x}})} \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(t, \hat{\mathbf{x}}) \right) + V(\hat{\mathbf{x}}). \quad (1)$$

Here, $V(\mathbf{x})$ stands for the associated scalar potential, and the meaning of all the other symbols is self-evident.

The purpose of the present paper is to switch from the MG into the acceleration gauge (AG), which, in the case of a constant mass, has been often preferred in numerous past studies of matter-light interaction both for conceptual and practical purposes, as already pointed out in the Introduction. In Sec. III A below, the passage from the MG into AG is performed in a self-contained manner within the classical mode of description, and canonical quantization is applied subsequently. The resulting AG Hamiltonian is then found to be

$$\begin{aligned} \hat{H}_{\text{AG}}(t) = & \frac{\hat{\mathbf{p}}^T \cdot \mathbb{Q}^T(t, \hat{\mathbf{y}}) \cdot \mathbb{Q}(t, \hat{\mathbf{y}}) \cdot \hat{\mathbf{p}}}{2m(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}}))} + V(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}})) \\ & + \frac{q^2}{2m(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}}))c^2} A^2(t, \hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}})) + \widehat{\text{QM}} \end{aligned} \quad (2)$$

[see Eq. (37) of Sec. III]. Here, $\hat{\mathbf{y}}$ represents the AG position operator, $\hat{\mathbf{p}}$ the associated canonical momentum, and $\mathbf{F}(t, \mathbf{y})$ plays the role of the Kramers-Henneberger (KH) quiver amplitude [1,5]. In the rather general setting presented here (when the mass is allowed to be more or less arbitrarily position dependent, and when even the dipole approximation is not imposed), the entity $\mathbf{F}(t, \mathbf{y})$ is obtainable by solving the following initial value problem,

$$\begin{aligned} \partial_t \mathbf{F}(t, \mathbf{y}) = & - \frac{q}{m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c} \mathbf{A}(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})), \\ \mathbf{F}(t \rightarrow -\infty, \mathbf{y}) = & \mathbf{0} \end{aligned} \quad (3)$$

[see Eqs. (30) and (31) of Sec. III]. Prescription (3) needs to be recognized as an ordinary (nonlinear) differential equation for $\mathbf{F}(t, \mathbf{y})$, in which t is the relevant active variable, and the spatial location \mathbf{y} stands just for a fixed parameter. Entity $\mathbb{Q}(t, \mathbf{y})$ appearing in (2) should be understood as an inverse of a 3×3 Jacobian matrix $\mathbb{G}(t, \mathbf{y})$ with elements $G_{jj'}(t, \mathbf{y}) = \delta_{jj'} + \partial_j F_{j'}(t, \mathbf{y})$. Finally, the as yet undetermined last term $\widehat{\text{QM}}$ of (2) compensates formally for the possibly improper operator ordering, and makes thus $\hat{H}_{\text{AG}}(t)$ [of Eq. (2)] the unitary equivalent to $\hat{H}_{\text{MG}}(t)$ [of Eq. (1)]. Clearly, $\widehat{\text{QM}}$ is of a purely quantum mechanical origin, and it becomes irrelevant in the classical limit. An explicit form of $\widehat{\text{QM}}$ will be given below in Sec. II B under some additional simplifying assumptions [see Eq. (7)].

B. One-dimensional systems, and weak-field regime under the dipole approximation

More explicit insights into the studied problem can be obtained in the one-dimensional case, while assuming the regime of weak-field intensities and while imposing the dipole approximation. The MG Hamiltonian $\hat{H}_{\text{MG}}(t)$ of Eq. (1) is

simplified accordingly, into

$$\hat{H}_{\text{MG}}(t) = \hat{p} \frac{1}{2m(\hat{x})} \hat{p} - \frac{q}{2c} A(t) \left\{ \frac{1}{m(\hat{x})} \hat{p} + \hat{p} \frac{1}{m(\hat{x})} \right\} + V(\hat{x}). \quad (4)$$

The corresponding AG Hamiltonian $\hat{H}_{\text{AG}}(t)$ of Eq. (2) possesses then the following appearance,

$$\hat{H}_{\text{AG}}(t) = \hat{p} \frac{1}{2m(\hat{y} - \mathbf{F}(t, \hat{y}))} \hat{p} + V(\hat{y} + \mathbf{F}(t, \hat{y})) + \widehat{\text{QM}} \quad (5)$$

[see Eq. (67) of Sec. III]. Here, the associated KH quiver amplitude $F(t, y)$ is given by an explicit formula

$$F(t, y) = - \frac{q}{m(y)c} \int_{-\infty}^t A(\tau) d\tau \quad (6)$$

[see Eq. (44) of Sec. III]. Moreover, the peculiar quantum mechanical $\widehat{\text{QM}}$ term comes out explicitly as

$$\widehat{\text{QM}} = \frac{\hbar^2}{4} \left(\frac{F''(t, y)}{m(y)} \right)', \quad (7)$$

with the prime superscript standing for the spatial derivative ∂_y [see Eq. (68) of Sec. III]. Our above displayed AG Hamiltonian $\hat{H}_{\text{AG}}(t)$ of Eq. (5) is the unitary equivalent to $\hat{H}_{\text{MG}}(t)$ of Eq. (4) up to the leading order $\mathcal{O}(\varepsilon_0)$ of the maximum electric field amplitude ε_0 (see Secs. III B 2, IV A, and IV B for details). Before proceeding further, let us point out that the mass term $m(\hat{y} - \mathbf{F}(t, \hat{y}))$ of Eq. (5) contains a minus sign, as opposed to the mass term $m(\hat{y} + \mathbf{F}(t, \hat{y}))$ of Eq. (2). This sign difference arises due to terms brought in by the Jacobian matrix $\mathbb{Q}(t, \hat{\mathbf{y}})$ in the weak-field regime [see Sec. III B 1 below and especially Eq. (46); cf. also Eqs. (65) and (66) of Sec. III B 2].

C. Illustrative numerical examples

The physical equivalence of the above presented Hamiltonian formulas (4) and (5) is tested by investigating numerically the phenomenon of resonant tunneling of an electron through a pair of potential barriers in the presence of a monochromatic weak intensity laser light. The employed formalism of complex scaled scattering theory is essentially the same as in our previous work [2] (see also the corresponding Supplemental Material). There is only one substantial difference, namely, in our present paper, the mass $m(y)$ depends explicitly upon position, and this highly nontrivial fact needs to be properly accounted for, either via the standard MG Hamiltonian $\hat{H}_{\text{MG}}(t)$ of Eq. (4), or through our AG Hamiltonian $\hat{H}_{\text{AG}}(t)$ of Eq. (5) displayed above.

Figure 1 presents the results of our first example calculation. The upper panel shows the used double-barrier potential $V(x)$, which is similar as in Ref. [2]. The middle panel depicts the chosen profile of the position-dependent mass $m(x)$. One can see that $m(x)$ varies with x in much the same manner as $V(x)$ (see Sec. IV C for explicit details). Such a choice of $m(x)$ is consistent with a physically motivated assumption that both $V(x)$ and $m(x)$ are determined by the local composition of the semiconductor material inside which the electron is set to move [3,4]. Note also that the asymptotic region of $x \rightarrow \pm\infty$ corresponds to a constant (spatially homogeneous) semiconductor. This is why $m(x \rightarrow \pm\infty)$ approaches a constant value

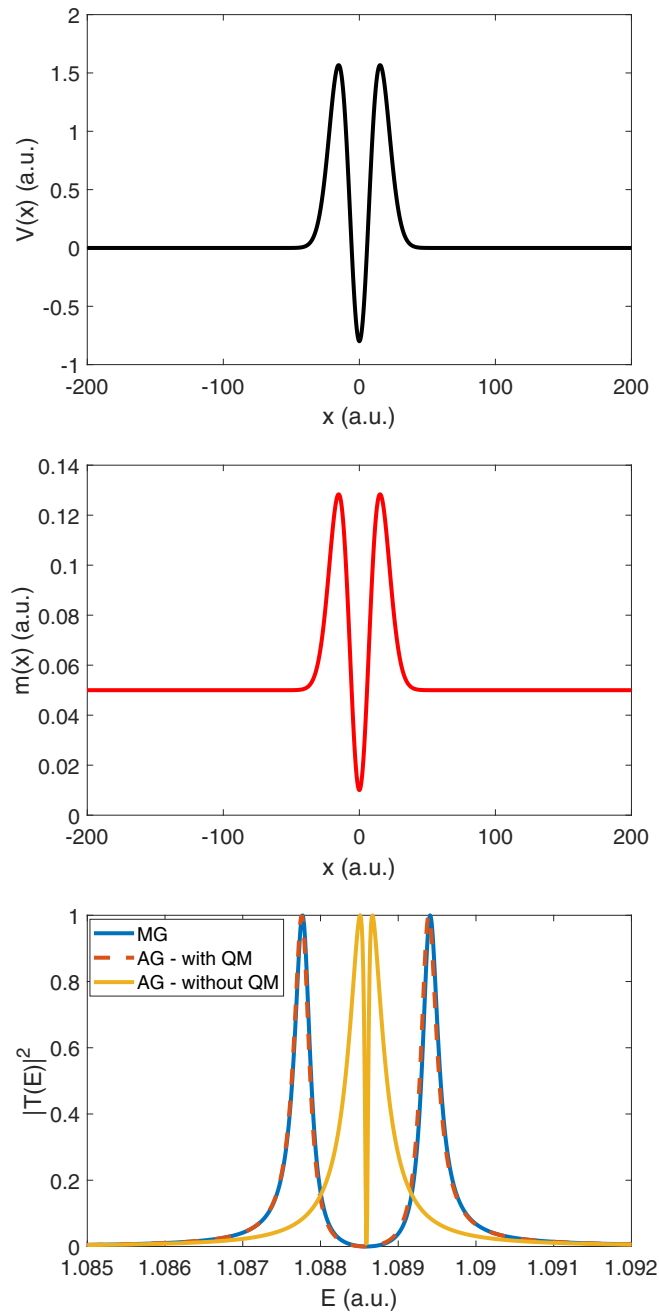


FIG. 1. Numerical illustration of physical equivalence between the MG and AG Hamiltonians (4) and (5). Upper panel: The used potential function $V(x)$. Middle panel: The used mass function $m(x)$. Lower panel: The corresponding transmission probability $|T(E)|^2$ plotted as a function of energy E of the incoming electron. More details regarding the system parameters can be found in Sec. IV.

which still differs from the usual mass of an electron in free space. The lower panel of Fig. 1 depicts then the obtained transmission probability $|T(E)|^2$ plotted as a function of the incident energy E of the electron. Most importantly, the blue line profile of $|T(E)|^2$, calculated using the MG Hamiltonian $\hat{H}_{MG}(t)$ of Eq. (4), agrees almost exactly with the dashed red line outcome, which is based upon the AG Hamiltonian $\hat{H}_{AG}(t)$ of Eq. (5). A tiny but visible difference between the

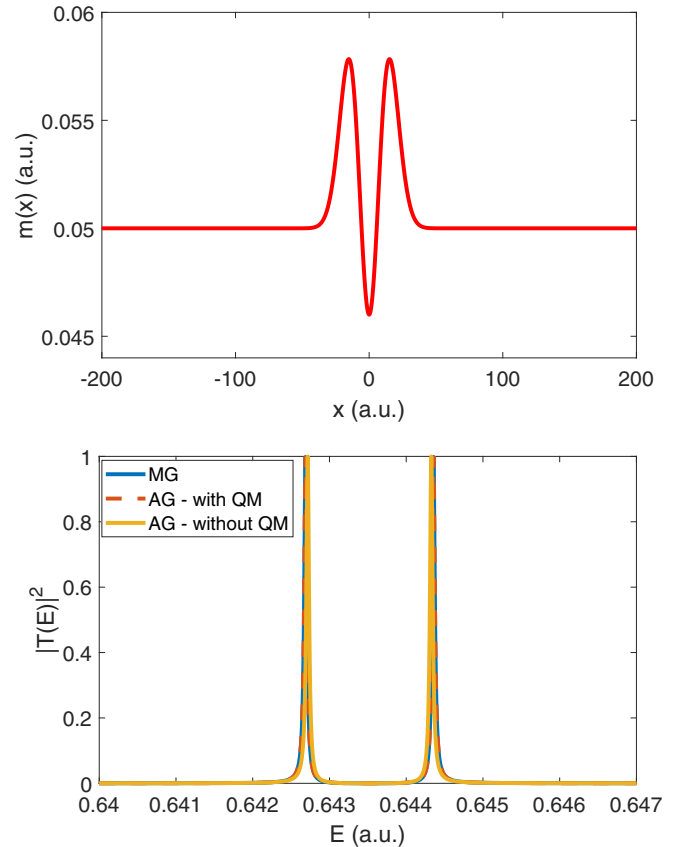


FIG. 2. Another numerical illustration of physical equivalence between the MG and AG Hamiltonians (4) and (5). The potential $V(x)$ is the same as in Fig. 1. Upper panel: The used mass function $m(x)$, varying now substantially less along x compared to the case of Fig. 1. Lower panel: The corresponding transmission probability $|T(E)|^2$ plotted as a function of energy E of the incoming electron. More details regarding the system parameters can be found in Sec. IV.

MG and AG results is most likely attributable to the weak-field assumption inherent in $\hat{H}_{AG}(t)$. In addition, and most importantly, the solid yellow line of Fig. 1 demonstrates that the purely quantum mechanical contribution QM [of Eq. (7)] to $\hat{H}_{AG}(t)$ cannot be ignored, since it affects crucially the resulting profile of $|T(E)|^2$. More details regarding the system parameters and the computational method are conveniently relegated to Sec. IV.

Our second illustrative calculation is presented in Fig. 2. We have implemented only a single modification of the system parameters of Fig. 1, namely, the used mass function $m(x)$ varies now substantially less with x compared to the $m(x)$ of Fig. 1. Note also that the asymptotic mass value $m(x \rightarrow \pm\infty)$ remains the same as in Fig. 1. As the x variation of $m(x)$ becomes weaker, the magnitude of the Hamiltonian term QM of Eq. (7) is scaled down accordingly, hence also the physical fingerprints of QM are expected to become less significant. Figure 2 neatly confirms this anticipation, showing that QM can actually be neglected, almost without changing the resulting outcome $|T(E)|^2$. Additional details, including more plots, are again relegated to Sec. IV.

III. SELF-CONTAINED DERIVATION OF THE ACCELERATION-GAUGE HAMILTONIAN

A. The general acceleration-gauge Hamiltonian

1. Starting point

Let us consider a charged nonrelativistic classical particle living in three spatial dimensions. This particle is assumed to possess a position-dependent mass $m(\mathbf{x})$, and it is exposed to an action of an external potential $V(\mathbf{x})$, as well as to driving by an externally prescribed classical electromagnetic field $\mathbf{A}(t, \mathbf{x})$ (e.g., by a laser pulse). The just presented classical problem is characterized by the following standard¹ Lagrangian [11],

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2}m(\mathbf{x})\dot{\mathbf{x}}^2 - V(\mathbf{x}) + \frac{q}{c}\mathbf{A}(t, \mathbf{x}) \cdot \dot{\mathbf{x}}, \quad (8)$$

where the overdot denotes the time derivative. The meaning of all the other involved symbols should be self-evident. We do not invoke the dipole approximation here. Proceeding towards the Hamiltonian formalism in standard fashion [12], we define the canonical momentum conjugate \mathbf{P} of \mathbf{x} , by the formula

$$P_j = \frac{\partial L}{\partial \dot{x}^j} = m(\mathbf{x})\dot{x}^j + \frac{q}{c}A_j(t, \mathbf{x}), \quad (9)$$

then also

$$\dot{x}^j = \frac{1}{m(\mathbf{x})} \left(P^j - \frac{q}{c}A^j(t, \mathbf{x}) \right). \quad (10)$$

The corresponding Hamiltonian is subsequently obtained via the Legendre transform,

$$H_{MG}(t) = \dot{x}^j P_j - L = \frac{1}{2m(\mathbf{x})} \left(\mathbf{P} - \frac{q}{c}\mathbf{A}(t, \mathbf{x}) \right)^2 + V(\mathbf{x}). \quad (11)$$

This is of course the well-known momentum-gauge (MG) Hamiltonian [11].

2. Passage to the acceleration gauge: Coordinate transformation

Our goal is to invent now the passage from the MG into the acceleration gauge (AG), while taking into account the already discussed spatial dependence of the mass $m(\mathbf{x})$, and without imposing any additional simplifying assumptions (in particular, without resorting to the dipole approximation). We shall start our elaborations by carrying out a coordinate transformation

$$\mathbf{x} = \mathbf{y} + \mathbf{F}(t, \mathbf{y}), \quad (12)$$

in analogy to the original work of Kramers and Henneberger [1]. Here, \mathbf{y} represents the AG spatial coordinate, and the entity $\mathbf{F}(t, \mathbf{y})$ (to be called the quiver amplitude in conformity with usual practice [1,5]) stands for an as yet unspecified function of space and time, confined only by the requirement of invertibility of formula (12). Clearly, prescription (12) establishes a bijective correspondence $\mathbf{x} \leftrightarrow \mathbf{y}$ if the Jacobian matrix $\mathbb{G}(t, \mathbf{y})$, with elements

$$G_{j'j}(t, \mathbf{y}) = \frac{\partial x^j}{\partial y^{j'}} = \delta_{jj'} + \partial_{j'}F_j(t, \mathbf{y}), \quad (13)$$

is always regular at all locations \mathbf{y} , i.e., if

$$\det \mathbb{G}(t, \mathbf{y}) \neq 0 \quad (\forall t \in \mathbb{R})(\forall \mathbf{y} \in \mathbb{R}^3). \quad (14)$$

Condition (14) is obviously satisfied as long as all the spatial derivatives $\partial_{j'}F_j(t, \mathbf{y})$ are small enough in magnitude; we shall return to this issue later on at the end of Sec. III A 4. For our forthcoming purposes, it is convenient to define at this point also the inverse Jacobian matrix

$$\mathbb{Q}(t, \mathbf{y}) = \mathbb{G}^{-1}(t, \mathbf{y}). \quad (15)$$

The corresponding matrix elements

$$Q^{jj'}(t, \mathbf{y}) = \frac{\partial y^{j'}}{\partial x^j} \quad (16)$$

can be worked out analytically using (13) if needed.

3. Passage to the acceleration gauge: Elaborations

The differentiation of Eq. (12) with respect to time yields

$$\dot{\mathbf{x}} = \dot{\mathbf{y}} + \dot{\mathbf{F}}(t, \mathbf{y}) + \partial_j \mathbf{F}(t, \mathbf{y}) \dot{y}^j. \quad (17)$$

We have conveniently adopted here the Einstein summation convention (one performs a summation over each pair of repeated indices). Correspondingly, the Lagrangian (8) can be transformed into an equivalent appearance

$$\begin{aligned} L(\mathbf{y}, \dot{\mathbf{y}}) &= \frac{1}{2}m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))(\dot{\mathbf{y}} + \dot{\mathbf{F}}(t, \mathbf{y}) \\ &\quad + \partial_j \mathbf{F}(t, \mathbf{y}) \dot{y}^j)^2 - V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &\quad + \frac{q}{c}\mathbf{A}(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \cdot (\dot{\mathbf{y}} + \dot{\mathbf{F}}(t, \mathbf{y}) + \partial_j \mathbf{F}(t, \mathbf{y}) \dot{y}^j). \end{aligned} \quad (18)$$

Proceeding towards the Hamiltonian formalism in standard fashion [12], we define the canonical momentum conjugate \mathbf{p} of \mathbf{y} , by formula

$$\begin{aligned} p_j &= \frac{\partial L}{\partial \dot{y}^j} \\ &= m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))(\dot{y}^j + \dot{F}^j(t, \mathbf{y}) + \partial_{j'}F^j(t, \mathbf{y})\dot{y}^{j'}) \\ &\quad \times (\delta_{jj'} + \partial_j F_{j'}(t, \mathbf{y})) \\ &\quad + \frac{q}{c}A^j(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y}))(\delta_{jj'} + \partial_j F_{j'}(t, \mathbf{y})) \\ &= m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))(\dot{y}^j + \dot{F}^j(t, \mathbf{y}) \\ &\quad + \partial_{j'}F^j(t, \mathbf{y})\dot{y}^{j'})G_{jj'}(t, \mathbf{y}) \\ &\quad + \frac{q}{c}A^j(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y}))G_{jj'}(t, \mathbf{y}). \end{aligned} \quad (19)$$

Note that p_j refers to the j th Cartesian component of the canonical momentum in the AG representation. On the other hand, the previously encountered symbol P_j refers to the j th Cartesian component of the canonical momentum in the MG representation. Equation (19) is equivalent to

$$\begin{aligned} Q^{jj'}(t, \mathbf{y})p_{j'} &= m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))(\dot{y}^j + \dot{F}^j(t, \mathbf{y}) + \partial_{j'}F^j(t, \mathbf{y})\dot{y}^{j'}) \\ &\quad + \frac{q}{c}A^j(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})). \end{aligned} \quad (20)$$

Hence also

$$\begin{aligned} m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \left\{ Q^{jj'}(t, \mathbf{y})p_{j'} - \frac{q}{c}A^j(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\} \\ = \dot{y}^j + \dot{F}^j(t, \mathbf{y}) + \partial_{j'}F^j(t, \mathbf{y})\dot{y}^{j'}, \end{aligned} \quad (21)$$

¹This is standard except for including the spatially dependent mass.

and subsequently

$$\begin{aligned} \dot{y}^j &= m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))Q_{j'}^j(t, \mathbf{y}) \\ &\times \left\{ Q^{j'j''}(t, \mathbf{y})p_{j''} - \frac{q}{c}A^{j'}(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\} \\ &- Q_{j'}^j(t, \mathbf{y})\dot{F}^{j'}(t, \mathbf{y}). \end{aligned} \quad (22)$$

To simplify our subsequent notations, let us conveniently adopt another shorthand symbol,

$$\wp^{jj'} = Q^{jj'}(t, \mathbf{y})p_{j'}, \quad (23)$$

such that

$$\wp = \mathbb{Q}(t, \mathbf{y}) \cdot \mathbf{p}. \quad (24)$$

Recall that $\mathbb{Q}(t, \mathbf{y})$ represents the Jacobian matrix (15). Equations (21) and (22) can be now redisplayed as follows:

$$\begin{aligned} \dot{y}^j + \dot{F}^j(t, \mathbf{y}) + \partial_{j'}F^j(t, \mathbf{y})\dot{y}^{j'} \\ = m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \left\{ \wp^j - \frac{q}{c}A^j(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\}, \end{aligned} \quad (25)$$

and

$$\begin{aligned} \dot{y}^j &= m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))Q_{j'}^j(t, \mathbf{y}) \left\{ \wp^{jj'} - \frac{q}{c}A^{j'}(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\} \\ &- Q_{j'}^j(t, \mathbf{y})\dot{F}^{j'}(t, \mathbf{y}). \end{aligned} \quad (26)$$

The sought Hamiltonian is obtained again via the standard Legendre transform,

$$\begin{aligned} H_{\text{AG}}(t) &= \dot{y}^j p_j - L \\ &= m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))\wp \cdot \left\{ \wp - \frac{q}{c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\} \\ &- \wp \cdot \dot{\mathbf{F}}(t, \mathbf{y}) \\ &- \frac{1}{2}m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \left\{ \wp - \frac{q}{c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\}^2 \\ &+ V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &- \frac{q}{c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \cdot \left\{ \wp - \frac{q}{c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\} \\ &\times m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &= \frac{1}{2}m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \left\{ \wp - \frac{q}{c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \right\}^2 \\ &+ V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) - \wp \cdot \dot{\mathbf{F}}(t, \mathbf{y}). \end{aligned} \quad (27)$$

Clearly, $H_{\text{AG}}(t)$ of Eq. (27) reduces to $H_{\text{MG}}(t)$ of Eq. (11) if one sets $\mathbf{F}(t, \mathbf{y}) = \mathbf{0}$. Instead of (27) one may write more concisely

$$\begin{aligned} H_{\text{AG}}(t) &= \frac{\wp^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))} + V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &+ \frac{q^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c^2}A^2(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &- \frac{q}{c}m^{-1}(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))\wp \cdot A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &- \wp \cdot \dot{\mathbf{F}}(t, \mathbf{y}). \end{aligned} \quad (28)$$

4. Passage to the acceleration gauge: The AG quiver amplitude

The coordinate transformation (12) was so far left rather arbitrary, since the quiver amplitude $F(t, \mathbf{y})$ has not been specified. We shall finalize now the definition of AG by fixing $F(t, \mathbf{y})$ in such a particular way as to erase the second line of formula (28). In other words, we wish to erase all the Hamiltonian terms linear in the momentum \wp and to obtain simply

$$\begin{aligned} H_{\text{AG}}(t) &= \frac{\wp^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))} + V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) \\ &+ \frac{q^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c^2}A^2(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})). \end{aligned} \quad (29)$$

The just stated requirement is fulfilled if and only if $F(t, \mathbf{y})$ possesses the property

$$\dot{F}(t, \mathbf{y}) = -\frac{q}{m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c}A(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})). \quad (30)$$

Formula (30) needs to be understood as an ordinary (nonlinear) differential equation for $F(t, \mathbf{y})$, in which t is the relevant active variable, and \mathbf{y} stands just for a fixed parameter. As the physically appropriate initial condition we shall choose having

$$\mathbf{F}(t \rightarrow -\infty, \mathbf{y}) = \mathbf{0}, \quad (31)$$

such that $H_{\text{AG}}(t)$ of Eq. (29) reduces to the standard field-free Hamiltonian corresponding to the situation before the arrival of the laser pulse. The initial value problem (30) and (31) is always uniquely solvable for the sought AG quiver amplitude $F(t, \mathbf{y})$. An explicit solution can be accomplished either by numerical calculation, or through imposing additional assumptions and approximations as we do below in Secs. III A 6 and III B. In any case, Eq. (30) represents a natural generalization of its well-established counterpart corresponding to a constant mass [1,5].

Recall that $F(t, \mathbf{y})$ enters the Jacobian matrix $\mathbb{G}(t, \mathbf{y})$ through (13). Thus the Jacobian (14) depends continuously upon the laser field profile experienced by the particle since the arrival of the pulse until the considered time instant t . We may thus infer that the Jacobian (14) remains nonzero and positive at least as long as the maximum laser field amplitude ε_0 does not exceed a certain threshold value $\varepsilon_0^{\text{max}}$ (which would undoubtedly depend both upon other parameters of the laser pulse and upon the studied system). It is not the scope of the present work to search for any encounter of the singular situation $\det \mathbb{G}(t, \mathbf{y}) = 0$. However, it might be worth keeping in mind that the possibility of having either $\det \mathbb{G}(t, \mathbf{y}) = 0$ or $\det \mathbb{G}(t, \mathbf{y}) \doteq 0$ has not been *a priori* excluded, and that another kind of interesting physics may arguably pop out under such circumstances.

5. Passage to the acceleration gauge: The AG Hamiltonian

Having in hand the just discussed AG quiver amplitude $F(t, \mathbf{y})$ satisfying presumably the regularity condition (14), we are ready to write down the final result for the sought classical AG Hamiltonian $H_{\text{AG}}(t)$. A combination of (32) and

(24) yields a compelling expression,

$$H_{AG}(t) = \frac{\mathbf{p}^T \cdot \mathbb{Q}^T(t, \mathbf{y}) \cdot \mathbb{Q}(t, \mathbf{y}) \cdot \mathbf{p}}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))} + V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) + \frac{q^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c^2} A^2(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})). \quad (32)$$

Here, $\mathbb{Q}(t, \mathbf{y})$ is the Jacobian matrix (15) with elements (16). At the classical level of theory, the Hamiltonian $H_{AG}(t)$ of Eq. (32) is exactly equivalent to its momentum-gauge counterpart $H_{MG}(t)$ of Eq. (11). Note that the kinetic term of (32) is an off-diagonal quadratic form in the momentum components. Note also the presence of the A^2 term, playing the role of an additional light-induced potential.

6. Special case: Position-independent mass, and dipole approximation

Substantial simplifications result in the case when the mass m does not depend upon \mathbf{x} and when the dipole approximation is adopted. Namely, Eq. (30) boils down into

$$\dot{\mathbf{F}}(t) = -\frac{q}{mc} \mathbf{A}(t), \quad (33)$$

hence

$$\mathbf{F}(t) = -\frac{q}{mc} \int_{-\infty}^t \mathbf{A}(\tau) d\tau. \quad (34)$$

Formula (34) is recognized immediately as the conventional AG quiver amplitude known in the literature [1,5]. Subsequently, the Jacobian matrix $\mathbb{Q}(t, \mathbf{y})$ of Eq. (15) reduces to unity, simply because $\mathbf{x} = \mathbf{y} + \mathbf{F}(t)$. Correspondingly, the Hamiltonian (32) becomes just

$$H_{AG}(t) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{y} + \mathbf{F}(t)), \quad (35)$$

again in full conformity with the standard literature [1,5].

7. Quantization

Canonical quantization of the studied problem runs along standard lines both in MG and AG, modulo the operator ordering controversy to be encountered and addressed shortly. The pertinent canonical commutation rules are of course $[\hat{x}^j, \hat{p}_j] = \delta_{jj'} i\hbar \hat{1}$ (MG), and $[\hat{y}^j, \hat{p}_j] = \delta_{jj'} i\hbar \hat{1}$ (AG). The MG Hamiltonian $H_{MG}(t)$ of Eq. (11) needs to be promoted accordingly to a Hermitian operator, yet such a promotion step is apparently ambiguous, since an ordering of the involved operators $[\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(t, \hat{\mathbf{x}})]$ and $\frac{1}{2m(\hat{\mathbf{x}})}$ is left *a priori* unspecified. In the present paper, we shall adhere to an already well-established ordering prescription (justified and used in Refs. [3])² by setting

$$\hat{H}_{MG}(t) = \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(t, \hat{\mathbf{x}}) \right) \frac{1}{2m(\hat{\mathbf{x}})} \left(\hat{\mathbf{p}} - \frac{q}{c} \mathbf{A}(t, \hat{\mathbf{x}}) \right) + V(\hat{\mathbf{x}}). \quad (36)$$

²The first reference quoted in Ref. [3] shows that other operator orderings lead either to divergence or to the nonuniqueness of the Hamiltonian eigenvalues. Hence these other operator orderings lack physical meaning.

A similar kind of operator ordering controversy persists also in the case of the AG Hamiltonian $H_{AG}(t)$ of Eq. (32). We shall thus write for now

$$\hat{H}_{AG}(t) = \frac{\hat{\mathbf{p}}^T \cdot \mathbb{Q}^T(t, \hat{\mathbf{y}}) \cdot \mathbb{Q}(t, \hat{\mathbf{y}}) \cdot \hat{\mathbf{p}}}{2m(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}}))} + V(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}})) + \frac{q^2}{2m(\hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}}))c^2} A^2(t, \hat{\mathbf{y}} + \mathbf{F}(t, \hat{\mathbf{y}})) + \widehat{\mathbb{Q}\mathbb{M}}, \quad (37)$$

where the as yet undetermined Hermitian operator $\widehat{\mathbb{Q}\mathbb{M}}$ compensates formally for the possibly improper operator ordering in the first line, and arranges thereby for an unitary equivalence between $\hat{H}_{AG}(t)$ [of Eq. (37)] and $\hat{H}_{MG}(t)$ [of Eq. (36)]. Taking into consideration our above-described classical transformation from the MG into the AG, one may seriously doubt whether it is possible to find any general and closed-form expression for $\widehat{\mathbb{Q}\mathbb{M}}$. Clearly, $\widehat{\mathbb{Q}\mathbb{M}}$ vanishes identically under the dipole approximation in the case of a position-independent mass, since the problem simplifies exactly as above in Sec. III A 7. When the spatial dependence of the mass comes into play and/or when the dipole approximation is not made, one may think of two promising ways of accessing $\widehat{\mathbb{Q}\mathbb{M}}$. (i) Via repeating the derivation pursued above in Secs. III A 1–III A 6, but now within the quantum mechanical framework, where all the operator noncommutativities are accounted for explicitly in the form of an \hbar expansion: This would lead towards developing a power series for $\widehat{\mathbb{Q}\mathbb{M}}$ whose terms need to be evaluated sequentially order by order. We do not pursue such an approach in the present paper. (ii) Via examining only the weak-field intensity regime within the dipole approximation, where such developments are relegated to a separate Sec. III B and lead towards a simple closed formula for $\widehat{\mathbb{Q}\mathbb{M}}$.

B. Special form of the AG Hamiltonian: Weak-field regime, dipole approximation, and one spatial dimension

For the sake of maximum simplicity, and also as a preparation for our illustrative numerical calculations pursued in Sec. IV, we shall hereafter restrict ourselves to studying the particle motion in one spatial dimension only. However, all the elaborations presented below are rather trivially generalizable to the three-dimensional case.

1. Classical treatment followed by formal quantization

In one spatial dimension, the classical Hamiltonian formulas (11) and (32) boil down into

$$H_{MG}(t) = \frac{1}{2m(x)} \left(P - \frac{q}{c} A(t, x) \right)^2 + V(x), \quad (38)$$

and

$$H_{AG}(t) = \frac{p^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))(1 + F'(t, \mathbf{y}))^2} + V(\mathbf{y} + \mathbf{F}(t, \mathbf{y})) + \frac{q^2}{2m(\mathbf{y} + \mathbf{F}(t, \mathbf{y}))c^2} A^2(t, \mathbf{y} + \mathbf{F}(t, \mathbf{y})). \quad (39)$$

For the sake of clarity, we note explicitly in this context that $\mathbb{G}(t, \mathbf{y}) = [1 + F'(t, \mathbf{y})]$, where the prime superscript stands for ∂_y . Let us assume in addition a weak-field regime, meaning

that all the terms higher than linear in the maximum electric field strength ε_0 will be hereafter neglected in the Hamiltonian. The A^2 term disappears then from (38) and (39), giving

$$H_{\text{MG}}(t) = \frac{P^2}{2m(x)} - \frac{q}{m(x)c} A(t,x)P + V(x), \quad (40)$$

and

$$H_{\text{AG}}(t) = \frac{p^2}{2m(y + F(t,y))(1 + F'(t,y))^2} + V(y + F(t,y)). \quad (41)$$

Let us impose also the dipole approximation, such that $A(t,x) \doteq A(t)$. Then

$$H_{\text{MG}}(t) = \frac{P^2}{2m(x)} - \frac{q}{m(x)c} A(t)P + V(x). \quad (42)$$

Under the dipole approximation, formula (30) boils down into

$$\dot{F}(t,y) = -\frac{q}{m(y + F(t,y))c} A(t), \quad (43)$$

or even to $\dot{F}(t,y) = -\frac{q}{m(y)c} A(t)$ for weak fields. Correspondingly, our AG quiver amplitude is equal to

$$F(t,y) = -\frac{q}{c m(y)} \int_{-\infty}^t A(t') dt', \quad (44)$$

in close resemblance to Eq. (34). Subsequently we have also

$$F'(t,y) = -\frac{m'(y)}{m(y)} F(t,y). \quad (45)$$

If so, one may recognize that

$$\begin{aligned} & m(y + F(t,y))(1 + F'(t,y))^2 \\ &= m(y) + m'(y)F(t,y) + 2m(y)F'(t,y) \\ &= m(y) - m'(y)F(t,y) = m(y - F(t,y)), \end{aligned} \quad (46)$$

valid again in the weak-field regime where only the terms linear in F are retained. Our resulting simplified AG Hamiltonian reads then as follows:

$$H_{\text{AG}}(t) = \frac{p^2}{2m(y - F(t,y))} + V(y + F(t,y)). \quad (47)$$

Interestingly, the denominator of the kinetic term contains $m(y - F(t,y))$, contrary to Eq. (32) where one finds $m(y + F(t,y))$. The minus sign appears in (47) due to an effect of $\mathbb{Q}(t,y) = [1 + F'(t,y)]^{-1}$, as detailed above in (46).

Having in hand $H_{\text{MG}}(t)$ [of Eq. (42)] and $H_{\text{AG}}(t)$ [of Eq. (47)], we are ready to carry out the formal canonical quantization exactly as described in Sec. III A 7. For $\hat{H}_{\text{MG}}(t)$ we adopt the same operator ordering as in Eq. (36), thus

$$\hat{H}_{\text{MG}}(t) = \hat{P} \frac{1}{2m(\hat{x})} \hat{P} - \frac{q}{2c} A(t) \left\{ \hat{P} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{P} \right\} + V(\hat{x}), \quad (48)$$

of course with $[\hat{x}, \hat{P}] = i\hbar \hat{1}$. In the case of AG we adhere to the attitude of Eq. (37), and set

$$\hat{H}_{\text{AG}}(t) = \hat{p} \frac{1}{2m(\hat{y} - F(t,\hat{y}))} \hat{p} + V(\hat{y} + \hat{F}(t,\hat{y})) + \widehat{\mathbb{Q}\mathbb{M}}, \quad (49)$$

of course with $[\hat{y}, \hat{p}] = i\hbar \hat{1}$. The extra $\widehat{\mathbb{Q}\mathbb{M}}$ term compensates here again for the possibly improper operator ordering, and arranges thereby for an unitary equivalence between $\hat{H}_{\text{AG}}(t)$ [of Eq. (49)] and $\hat{H}_{\text{MG}}(t)$ [of Eq. (48)]. An explicit form of $\widehat{\mathbb{Q}\mathbb{M}}$ cannot be accessed via the just outlined formal quantization of the classical AG Hamiltonian. In order to find $\widehat{\mathbb{Q}\mathbb{M}}$, we shall implement a direct quantum mechanical passage from the MG to AG, which is elaborated below in Sec. III B 2 while taking an enormous advantage of the two simplifying assumptions made above (weak-field regime, dipole approximation).

2. Direct quantum mechanical treatment

The starting point of our direct quantum mechanical treatment is given by the MG Hamiltonian $\hat{H}_{\text{MG}}(t)$ of Eq. (48). This Hamiltonian governs the quantum dynamics of the studied particle by means of the time-dependent Schrödinger equation

$$i\hbar \partial_t |\psi_t\rangle = \hat{H}_{\text{MG}}(t) |\psi_t\rangle. \quad (50)$$

For notational reasons, we shall conveniently rename now the canonical pair (\hat{x}, \hat{P}) into (\hat{y}, \hat{p}) , such that

$$\hat{H}_{\text{MG}}(t) = \hat{p} \frac{1}{2m(\hat{y})} \hat{p} - \frac{q}{2c} A(t) \left\{ \hat{p} \frac{1}{m(\hat{y})} + \frac{1}{m(\hat{y})} \hat{p} \right\} + V(\hat{y}). \quad (51)$$

Passage into AG is facilitated by the unitary transformation

$$|\psi_t\rangle = \hat{U}(t) |\varphi_t\rangle, \quad (52)$$

where we set conveniently

$$\hat{U}(t) = e^{+\frac{i}{\hbar} \hat{S}(t)}, \quad (53)$$

and

$$\hat{S}(t) = \frac{q}{2c} \left\{ \frac{1}{m(\hat{y})} \hat{p} + \hat{p} \frac{1}{m(\hat{y})} \right\} \int_{-\infty}^t A(t') dt'. \quad (54)$$

Equations (53) and (54) are inspired by the well-established quantum mechanical approach corresponding to the case of a constant (position-independent) mass [5]. Note that $\hat{S}(t)$ is a Hermitian operator proportional to the maximum laser field intensity ε_0 . An alternative appearance of $\hat{S}(t)$ is also useful, namely,

$$\hat{S}(t) = -\frac{1}{2} [F(t,\hat{y}) \hat{p} + \hat{p} F(t,\hat{y})], \quad (55)$$

of course with $F(t,y)$ given by Eq. (44). The transformed state vector $|\varphi_t\rangle$ evolves in time according to the time-dependent Schrödinger equation

$$i\hbar \partial_t |\varphi_t\rangle = \hat{H}_{\text{AG}}(t) |\varphi_t\rangle, \quad (56)$$

where by definition

$$\hat{H}_{\text{AG}}(t) = \hat{U}^\dagger(t) \hat{H}_{\text{MG}}(t) \hat{U}(t) - i\hbar \hat{U}^\dagger(t) \partial_t \hat{U}(t). \quad (57)$$

What remains to be done is to work out $\hat{H}_{\text{AG}}(t)$ explicitly up to the leading order $O(\varepsilon_0^1)$. This is a purely technical, somewhat tedious, but feasible task.

Clearly, one has

$$\hat{U}(t) = \hat{1} + \frac{i}{\hbar} \hat{S}(t) + O(\varepsilon_0^2). \quad (58)$$

Any quantum mechanical operator \hat{Q} is thus converted by $\hat{U}(t)$ into

$$\hat{U}^\dagger(t)\hat{Q}\hat{U}(t) = \hat{Q} + \frac{i}{\hbar}\hat{Q}\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)\hat{Q} + O(\varepsilon_0^2). \quad (59)$$

Moreover,

$$\hat{U}^\dagger(t)(-i\hbar)\partial_t\hat{U}(t) = \dot{\hat{S}}(t) + O(\varepsilon_0^2). \quad (60)$$

Our transformed Hamiltonian $\hat{H}_{AG}(t)$ of Eq. (57) can be now expressed as

$$\begin{aligned} \hat{H}_{AG}(t) &= \hat{H}_t + \frac{i}{\hbar}\hat{H}_t\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)\hat{H}_t + \dot{\hat{S}}(t) + O(\varepsilon_0^2) \\ &= \hat{p}\frac{1}{2m(\hat{y})}\hat{p} + \frac{i}{\hbar}\hat{p}\frac{1}{2m(\hat{y})}\hat{p}\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)\hat{p}\frac{1}{2m(\hat{y})}\hat{p} \\ &\quad + V(\hat{y}) + \frac{i}{\hbar}V(\hat{y})\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)V(\hat{y}) + O(\varepsilon_0^2). \end{aligned} \quad (61)$$

The $\frac{(-q)}{2c}A(t)\{\frac{1}{m(\hat{y})}\hat{p} + \hat{p}\frac{1}{m(\hat{y})}\}$ part of $\hat{H}_{MG}(t)$ [Eq. (51)] has been exactly overcompensated here by $\dot{\hat{S}}(t)$. Straightforward (although tedious) calculations now yield

$$\frac{i}{\hbar}V(\hat{y})\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)V(\hat{y}) = V'(\hat{y})F(t, \hat{y}), \quad (62)$$

and, similarly,

$$\begin{aligned} &\frac{i}{\hbar}\hat{p}\frac{1}{2m(\hat{y})}\hat{p}\hat{S}(t) - \frac{i}{\hbar}\hat{S}(t)\hat{p}\frac{1}{2m(\hat{y})}\hat{p} \\ &= \hat{p}\frac{(-1)}{2m(\hat{y})}\left(F(t, \hat{y})\frac{m'(\hat{y})}{m(\hat{y})} + 2F'(t, \hat{y})\right)\hat{p} \\ &\quad + \frac{\hbar^2}{4}\left(\frac{F''(t, \hat{y})}{m(\hat{y})}\right)'. \end{aligned} \quad (63)$$

After plugging (62) and (63) into (61) one arrives at a simple looking explicit expression for $\hat{H}_{AG}(t)$. Namely, one finds that

$$\begin{aligned} \hat{H}_{AG}(t) &= \hat{p}\frac{1}{2M(t, \hat{y})}\hat{p} + V(\hat{y}) + V'(\hat{y})F(t, \hat{y}) \\ &\quad + \frac{\hbar^2}{4}\left(\frac{F''(t, \hat{y})}{m(\hat{y})}\right)' + O(\varepsilon_0^2), \end{aligned} \quad (64)$$

where by definition

$$M(t, \hat{y}) = m(\hat{y}) + m'(\hat{y})F(t, \hat{y}) + 2m(\hat{y})F'(t, \hat{y}). \quad (65)$$

For the sake of clarity and completeness, we note explicitly that the kinetic term of (64) has been obtained via the following sequence of manipulations:

$$\begin{aligned} &\frac{1}{m(\hat{y})}\left(\hat{1} - F(t, \hat{y})\frac{m'(\hat{y})}{m(\hat{y})} - 2F'(t, \hat{y})\right) \\ &= \frac{1}{m(\hat{y})\left(\hat{1} + F(t, \hat{y})\frac{m'(\hat{y})}{m(\hat{y})} + 2F'(t, \hat{y})\right)} + O(\varepsilon_0^2) \\ &= \frac{1}{M(t, \hat{y})} + O(\varepsilon_0^2). \end{aligned} \quad (66)$$

The mass term (65) can be recognized as the quantity encountered already in (46). We thus write accordingly $M(t, \hat{y}) =$

$m(\hat{y} - F(t, \hat{y}))$. Finally, we erase the $O(\varepsilon_0^2)$ term of (64), and redisplay $\hat{H}_{AG}(t)$ in its compact and compelling appearance,

$$\hat{H}_{AG}(t) = \hat{p}\frac{1}{2m(\hat{y} - F(t, \hat{y}))}\hat{p} + V(\hat{y} + F(t, \hat{y})) + \widehat{QM}, \quad (67)$$

where by definition

$$\widehat{QM} = \frac{\hbar^2}{4}\left(\frac{F''(t, \hat{y})}{m(\hat{y})}\right)'. \quad (68)$$

Recall that $F(t, y)$ is given by Eq. (44), and that the prime superscript stands here for the spatial derivative ∂_y .

Most importantly, the just obtained AG Hamiltonian $\hat{H}_{AG}(t)$ of Eq. (67) agrees exactly with the outcome (49) of our alternative derivation based upon classical mechanics. Yet the extra \widehat{QM} term is now explicitly determined by prescription (68). (Note that \widehat{QM} vanishes in the case of a position-independent mass, as it should.) The above-constructed AG Hamiltonian (67) is the unitary equivalent to its MG counterpart (51) up to the leading order $O(\varepsilon_0^1)$ of the laser field strength.³ The physical equivalence of the Hamiltonian prescriptions $\hat{H}_{AG}(t)$ [Eqs. (67) and (68)] and $\hat{H}_{MG}(t)$ [Eq. (51)] will be demonstrated further in Sec. IV by illustrative numerical calculations.

Before proceeding to Sec. IV, we note that the quantum mechanical treatment of the present Sec. III B 2 can be further extended to cover even such situations when quantum fields are involved. In such a case, our starting MG Hamiltonian (48) would be modified, via replacing $A(t)$ by the appropriate QED operator of the vector potential, and the standard QED Hamiltonian of the free quantized radiation field would be added. Subsequently, our transformation into AG would correspond to the Bloch-Nordsieck transformation (BNT), which represents the QED counterpart of the semiclassical AG transformation (an insightful application of the BNT approach to molecules in laser fields is worked out in Refs. [13]). An appropriate implementation of the BNT in the present context would, of course, need to account for the spatial dependence of the electronic mass. We shall not elaborate on the BNT explicitly in the present paper, since this would take us too far afield. We note, however, that such an explicit formulation of the BNT approach becomes physically relevant as soon as our studied system (an electron moving in a semiconductor nanostructure environment) is exposed to an inherently quantum (nonclassical) state of radiation (e.g., to a number state, or a squeezed quantum state of the photon field).

IV. NUMERICAL ILLUSTRATION: RESONANCE TRANSMISSION PHENOMENA

As already pointed out above, the purpose of Sec. IV is to provide a numerical example utilizing the above-derived AG

³Correspondingly, an inverse of the unitary transformation (57) converts $\hat{H}_{AG}(t)$ back to $\hat{H}_{MG}(t)$ of Eq. (51) only up to the leading order of the laser field strength. Of course, additional complicating terms do pop out in the transformed Hamiltonian when one looks at higher orders of ε_0 . These effects would need to be properly taken under control via an additional unitary transformation of order $O(\varepsilon_0^2)$ and higher.

Hamiltonian $\hat{H}_{AG}(t)$ given by formulas (67) and (68). We have chosen to examine here the phenomenon of resonant⁴ scattering of an electron through a semiconductor nanostructure.⁵ Note that the same problem was, for the case of a constant mass, thoroughly investigated in our recent contribution [2]. For the sake of comparison and clarity, we shall also include below an analogous calculation based solely upon the MG Hamiltonian $\hat{H}_{MG}(t)$ [of Eqs. (48) or (51)].

A. Scattering of an electron through a semiconductor nanostructure: Momentum-gauge formulation

We prefer to introduce the studied physical problem first in the MG representation. Let us consider an electron moving in a semiconductor nanostructure environment. The mentioned environment influences our electron in two distinct ways: (i) It generates an external potential $V(x)$, such as the one plotted in the upper panel of Fig. 1. (ii) It changes the bare electron mass into its effective (renormalized) position-dependent counterpart $m(x)$ (see the middle panel of Fig. 1 or the upper panel of Fig. 2). In addition, we shall assume that the electron is exposed to an external monochromatic laser light, of a given frequency ω and of a weak-field strength ε_0 (weak enough as to allow only single-photon exchange processes to significantly occur).

The adequate MG Hamiltonian takes the form (48), with $A(t) = c \alpha \sin(\omega t)$ and $\alpha = \frac{\varepsilon_0}{\omega}$, thus

$$\hat{H}_{MG}(t) = \hat{p} \frac{1}{2m(\hat{x})} \hat{p} - \frac{q}{2} \left\{ \hat{p} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{p} \right\} \alpha \sin(\omega t) + V(\hat{x}). \quad (69)$$

Since $\hat{H}_{MG}(t)$ of Eq. (69) is time periodic with the period $T = \frac{2\pi}{\omega}$, we shall take advantage of the Floquet theory [14], exactly as we did before in Ref. [2]. The corresponding Floquet Hamiltonian reads as

$$\hat{\mathcal{H}}_{MG} = \hat{p} \frac{1}{2m(\hat{x})} \hat{p} - \frac{q}{2} \left\{ \hat{p} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{p} \right\} \alpha \sin(\omega t) + V(\hat{x}) - i\hbar \frac{\partial}{\partial t}. \quad (70)$$

In the single-photon approximation (appropriate in the regime of small enough ε_0), the time coordinate $t \in [0, T]$ can be

⁴The term ‘‘resonant’’ emphasizes that scattering is controlled here by long-living quasibound states (resonances) of the studied system.

⁵The used model is based upon Refs. [4], especially upon the work of Goldzak *et al.* Using the single-band effective-mass approximation, we can interpret the energy difference between the conduction bands of each semiconductor layer as the potential for the electrons in the conduction band. Barriers are formed by semiconductor materials with a larger band gap, and a potential well is formed by a semiconductor material with a smaller band gap. When the potential has a well, it may support bound states (there is actually one bound state in our particular case). However, bound states do not influence the scattering phenomena, since any electronic wave packet entering the interaction region from spatial infinity is expressible solely as a linear combination of the scattering (continuum) states.

adequately covered using just two Fourier basis functions $\sqrt{\frac{\omega}{2\pi}} e^{+i0\omega t}$ and $\sqrt{\frac{\omega}{2\pi}} e^{+i1\omega t}$ (see Refs. [2,14,15] for details). The Floquet Hamiltonian (70) is converted accordingly into the following block matrix appearance,

$$\hat{\mathcal{H}}_{MG} = \begin{pmatrix} \hat{p} \frac{1}{2m(\hat{x})} \hat{p} + V(\hat{x}) & +\frac{q}{2} \left\{ \hat{p} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{p} \right\} \frac{\alpha}{2i} \\ -\frac{q}{2} \left\{ \hat{p} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{p} \right\} \frac{\alpha}{2i} & \hat{p} \frac{1}{2m(\hat{x})} \hat{p} + V(\hat{x}) + \hbar\omega \end{pmatrix}. \quad (71)$$

Here, the single entries are time independent, and act in the space of x -dependent wave functions. In the asymptotic regions of $x \rightarrow \pm\infty$, the electron mass is assumed to become constant, $m(x \rightarrow \pm\infty) = m_\infty$, and the potential $V(x)$ falls off to zero. Hence the Hamiltonian $\hat{\mathcal{H}}_{MG}$ of Eq. (71) reduces into

$$\hat{\mathcal{H}}_{MG}^0 = \begin{pmatrix} \frac{\hat{p}^2}{2m_\infty} & +\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} \\ -\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} & \frac{\hat{p}^2}{2m_\infty} + \hbar\omega \end{pmatrix}. \quad (72)$$

Equation (72) is recognized as the Floquet Hamiltonian of an electron which possesses a constant effective mass m_∞ and moves along x just under an influence of an external weak intensity monochromatic field $A(t) = c \alpha \sin(\omega t)$.

An eigenvalue problem of the asymptotic Floquet Hamiltonian $\hat{\mathcal{H}}_{MG}^0$ of Eq. (72) is analytically solvable. Namely, one has

$$\begin{pmatrix} \frac{\hat{p}^2}{2m_\infty} & +\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} \\ -\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} & \frac{\hat{p}^2}{2m_\infty} + \hbar\omega \end{pmatrix} e^{+ikx} \begin{pmatrix} 1 \\ \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \end{pmatrix} = \frac{\hbar^2 k^2}{2m_\infty} e^{+ikx} \begin{pmatrix} 1 \\ \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \end{pmatrix}, \quad (73)$$

and similarly

$$\begin{pmatrix} \frac{\hat{p}^2}{2m_\infty} & +\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} \\ -\frac{q}{m_\infty} \hat{p} \frac{\alpha}{2i} & \frac{\hat{p}^2}{2m_\infty} + \hbar\omega \end{pmatrix} e^{+ikx} \begin{pmatrix} \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \\ 1 \end{pmatrix} = \left(\frac{\hbar^2 k^2}{2m_\infty} + \hbar\omega \right) e^{+ikx} \begin{pmatrix} \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \\ 1 \end{pmatrix}. \quad (74)$$

Here, k stands for an arbitrary real parameter. Relations (73) and (74) are valid in the weak-field regime, i.e., up to $O(\varepsilon_0)$. The eigensolutions associated with Eqs. (73) and (74) are interpreted physically in terms of the ubiquitous Volkov states [16], i.e., in terms of the plane-wave states of an electron with momentum $\hbar k$ which is exposed to an external laser driving.⁶ Note also that the column vectors $(1, \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2})^T$ and $(\frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2}, 1)^T$ are unit normalized up to $O(\varepsilon_0)$.

Our interest consists in studying the transmission phenomena, where an incoming electron prepared in a given

⁶Stated more explicitly, the Schrödinger equation $i\hbar \partial_t \psi(t, x) = \frac{1}{2m_\infty} (\hat{p} - \frac{q}{c} A(t))^2 \psi(t, x)$ possesses particular solutions of the form $e^{-i\frac{\hbar^2 k^2}{2m_\infty} t} e^{+ikx} e^{+i\frac{q}{m_\infty c} \hbar k \int_0^t A(t') dt'} e^{-i\frac{q^2}{\hbar} \frac{1}{2m_\infty c^2} \int_0^t A^2(t') dt'}$. These so-called Volkov states make up a complete set on the space of x -dependent wave functions. The eigensolutions displayed above in (73) and (74) are nothing more than just the mentioned Volkov states, corresponding to $A(t) = c \alpha \sin(\omega t)$, and translated into the Floquet language while neglecting all the terms higher than $O(\varepsilon_0)$.

asymptotic Floquet-Volkov⁷ state,

$$|\phi_{\text{in}}^{\text{MG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2k}} e^{+ikx} \begin{pmatrix} 1 \\ \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \end{pmatrix} \quad (k > 0), \quad (75)$$

is affected by an interaction

$$\widehat{V}_{\text{MG}} = \widehat{\mathcal{H}}_{\text{MG}} - \widehat{\mathcal{H}}_{\text{MG}}^0 = \begin{pmatrix} \hat{P} \frac{1}{2m(\hat{x})} \hat{P} - \frac{\hat{P}^2}{2m_\infty} + V(\hat{x}) & + \frac{q}{2} \left\{ \hat{P} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{P} \right\} \frac{\alpha}{2i} - \frac{q}{m_\infty} \hat{P} \frac{\alpha}{2i} \\ - \frac{q}{2} \left\{ \hat{P} \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{P} \right\} \frac{\alpha}{2i} + \frac{q}{m_\infty} \hat{P} \frac{\alpha}{2i} & \hat{P} \frac{1}{2m(\hat{x})} \hat{P} - \frac{\hat{P}^2}{2m_\infty} + V(\hat{x}) \end{pmatrix}, \quad (76)$$

and is finally found in an outgoing Floquet-Volkov state,

$$|\phi_{\text{out}}^{\text{MG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2k}} e^{+ikx} \begin{pmatrix} 1 \\ \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-ik)}{2} \end{pmatrix}. \quad (77)$$

The other outgoing Floquet-Volkov channel,

$$|\phi_{\text{out}}^{\text{MG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2K}} e^{+iKx} \begin{pmatrix} \frac{q}{m_\infty} \frac{\alpha}{\omega} \frac{(-iK)}{2} \\ 1 \end{pmatrix}, \quad (78)$$

$$\frac{\hbar^2 K^2}{2m_\infty} = \frac{\hbar^2 k^2}{2m_\infty} - \hbar\omega,$$

is closed in the studied range of the electron impact energies, and can thus be ignored. Formulas (75) and (77) contain the usual energy normalization prefactor $\sqrt{\frac{m_\infty}{2\pi\hbar^2k}}$, and similarly (78) contains a factor $\sqrt{\frac{m_\infty}{2\pi\hbar^2K}}$ (see the Supplemental Material of Ref. [2] for more information). The studied transmission process is completely characterized by the corresponding transmission coefficients, and these are determined by the Lippmann-Schwinger formula

$$T_{\text{MG}}(E) = 1 - 2\pi i \langle \phi_{\text{out}}^{\text{MG}} | \widehat{V}_{\text{MG}} | \phi_{\text{in}}^{\text{MG}} \rangle + \widehat{V}_{\text{MG}} \frac{1}{E - \widehat{\mathcal{H}}_{\text{MG}} + i0_+} \widehat{V}_{\text{MG}} | \phi_{\text{in}}^{\text{MG}} \rangle \quad (79)$$

(see again Ref. [2] and its Supplemental Material for the underlying background). In Eq. (79), $E = \frac{\hbar^2 k^2}{2m_\infty}$ represents of course the (quasi)energy of the incoming electron state (75).

While the Lippmann-Schwinger formula (79) is physically appropriate for the scattering problem under our consideration, its practical application may become numerically challenging. For this reason, we follow Ref. [2] and refine slightly the formalism of the present Sec. IV A, by switching into an equivalent non-Hermitian mode of description. In the current context, the most convenient mathematical language (suitable for performing efficiently practical computations) seems to be the non-Hermitian scattering theory based upon the exterior complex scaling (ECS) [15]. The ECS technique replaces the physical real valued coordinate x by an equivalent contour $f(x)$ in the complex x plane, such that

$$f(x) = \begin{cases} -x_0 + (x + x_0)e^{+i\theta}, & x \leq -x_0, \\ x, & -x_0 \leq x \leq +x_0, \\ +x_0 + (x - x_0)e^{+i\theta}, & x \geq +x_0. \end{cases} \quad (80)$$

⁷We shall hereafter use the double-bracket notation $|\phi_{\text{in/out}}\rangle$ in order to emphasize that the relevant state vectors belong in an extended space of functions depending upon the coordinates (x, t) .

Here, $x_0 > 0$ stands for a cutoff parameter, whose value is chosen to be large enough so as to ensure that the interaction \widehat{V}_{MG} vanishes for $|x| \geq x_0$. The symbol θ stands for the ubiquitous complex scaling angle [15]. An implementation of the ECS leaves both $V(x)$ and $m(x)$ unchanged, since these entities vary with x only inside the interaction region of $-x_0 \leq x \leq +x_0$. On the other hand, the momentum operator is changed into $\hat{P}_f = \left(\frac{df(x)}{dx}\right)^{-1} \hat{P}$. Thus

$$\hat{P}_f = \begin{cases} e^{-i\theta} \hat{P}, & |x| > x_0, \\ \hat{P}, & |x| < x_0. \end{cases} \quad (81)$$

We relegate the reader to Ref. [15] for more details.

The ECS changes our Floquet Hamiltonian (71) into

$$\widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}} = \begin{pmatrix} \hat{P}_f \frac{1}{2m(\hat{x})} \hat{P}_f + V(\hat{x}) & + \frac{q}{2} \left\{ \hat{P}_f \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{P}_f \right\} \frac{\alpha}{2i} \\ - \frac{q}{2} \left\{ \hat{P}_f \frac{1}{m(\hat{x})} + \frac{1}{m(\hat{x})} \hat{P}_f \right\} \frac{\alpha}{2i} & \hat{P}_f \frac{1}{2m(\hat{x})} \hat{P}_f + V(\hat{x}) + \hbar\omega \end{pmatrix}, \quad (82)$$

where the superscript NH stands for non-Hermitian. On the other hand, the interaction term (76) remains unaltered, since it possesses nonzero values only in the interaction region of $|x| < x_0$. The Lippmann-Schwinger formula (79) is accordingly converted into

$$T_{\text{MG}}(E) = 1 - 2\pi i \langle \phi_{\text{out}}^{\text{MG}} | \widehat{V}_{\text{MG}} | \phi_{\text{in}}^{\text{MG}} \rangle + \widehat{V}_{\text{MG}} \frac{1}{E - \widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}}} \widehat{V}_{\text{MG}} | \phi_{\text{in}}^{\text{MG}} \rangle. \quad (83)$$

For the sake of completeness and clarity, we note explicitly in this context that no singularity is encountered in $(E - \widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}})^{-1}$, since all the (resonance and continuum) eigenvalues of the non-Hermitian Hamiltonian $\widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}}$ possess a negative imaginary part. Moreover, ECS does not alter the wave functions $|\phi_{\text{in/out}}^{\text{MG}}\rangle$ in the interaction region, thus these in/out states are left without modification in (83). Formulas (83), (82), and (76) lend themselves well to practical numerical calculations of $T_{\text{MG}}(E)$. Computational details will be given in Sec. IV C below.

B. Scattering of an electron through a semiconductor nanostructure: Acceleration-gauge formulation

In the case of the acceleration gauge, our starting Floquet Hamiltonian is obtained using the previously derived formulas (67), (44), and (68) of Sec. III. Since $A(t) = c\alpha \sin(\omega t) e^{-\zeta|t|} |_{\zeta \rightarrow +0}$, we have

$$F(t, y) = \frac{q}{m(y)\omega} \cos(\omega t). \quad (84)$$

Subsequently, one gets

$$\begin{aligned}\widehat{\mathcal{H}}_{\text{AG}} &= \widehat{p} \frac{1}{2m(\widehat{y} - F(t, \widehat{y}))} \widehat{p} + V(\widehat{y} + F(t, \widehat{y})) + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} - i\hbar \frac{\partial}{\partial t} \\ &= \widehat{p} \frac{1}{2m(\widehat{y})} \widehat{p} + \widehat{p} \frac{m'(\widehat{y})}{2m^3(\widehat{y})} \widehat{p} \frac{q\alpha}{\omega} \cos(\omega t) + V(\widehat{y}) + V'(\widehat{y}) \\ &\quad \times \frac{q}{m(\widehat{y})} \frac{\alpha}{\omega} \cos(\omega t) + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} - i\hbar \frac{\partial}{\partial t},\end{aligned}\quad (85)$$

$$\widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}} = \begin{pmatrix} \widehat{p}_f \frac{1}{2m(\widehat{y})} \widehat{p}_f + V(\widehat{y}) & \widehat{p}_f \frac{m'(\widehat{y})}{2m^3(\widehat{y})} \widehat{p}_f \frac{q\alpha}{\omega} \frac{1}{2} + V'(\widehat{y}) \frac{q}{m(\widehat{y})} \frac{\alpha}{\omega} \frac{1}{2} + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} \frac{1}{2} \\ \widehat{p}_f \frac{m'(\widehat{y})}{2m^3(\widehat{y})} \widehat{p}_f \frac{q\alpha}{\omega} \frac{1}{2} + V'(\widehat{y}) \frac{q}{m(\widehat{y})} \frac{\alpha}{\omega} \frac{1}{2} + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} \frac{1}{2} & \widehat{p}_f \frac{1}{2m(\widehat{y})} \widehat{p}_f + V(\widehat{y}) + \hbar\omega \end{pmatrix}.\quad (87)$$

We have already tacitly included here the ECS, similarly as in Sec. IV A. Accordingly, one has

$$\widehat{p}_f = \begin{cases} e^{-i\theta} \widehat{p}, & |x| > x_0, \\ \widehat{p}, & |x| < x_0. \end{cases}\quad (88)$$

Single entries of the matrix (87) are time independent, and act in the space of y -dependent wave functions. Our AG Floquet Hamiltonian $\widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$ of Eq. (87) becomes dramatically simplified for $y \rightarrow \pm\infty$, where the electron mass is assumed to become constant and the potential falls off to zero. Indeed, one encounters just a diagonal matrix,

$$\widehat{\mathcal{H}}_{\text{AG}}^{0,\text{NH}} = \begin{pmatrix} \frac{\widehat{p}_f^2}{2m_\infty} & 0 \\ 0 & \frac{\widehat{p}_f^2}{2m_\infty} + \hbar\omega \end{pmatrix}.\quad (89)$$

$$\widehat{\mathcal{V}}_{\text{AG}} = \widehat{\mathcal{H}}_{\text{AG}} - \widehat{\mathcal{H}}_{\text{AG}}^0 = \widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}} - \widehat{\mathcal{H}}_{\text{AG}}^{0,\text{NH}} = \begin{pmatrix} \widehat{p} \frac{1}{2m(\widehat{y})} \widehat{p} - \frac{\widehat{p}^2}{2m_\infty} + V(\widehat{y}) & \widehat{p} \frac{m'(\widehat{y})}{2m^3(\widehat{y})} \widehat{p} \frac{q\alpha}{\omega} \frac{1}{2} + V'(\widehat{y}) \frac{q}{m(\widehat{y})} \frac{\alpha}{\omega} \frac{1}{2} + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} \frac{1}{2} \\ \widehat{p} \frac{m'(\widehat{y})}{2m^3(\widehat{y})} \widehat{p} \frac{q\alpha}{\omega} \frac{1}{2} + V'(\widehat{y}) \frac{q}{m(\widehat{y})} \frac{\alpha}{\omega} \frac{1}{2} + \widehat{\mathcal{Q}}\widehat{\mathcal{M}} \frac{1}{2} & \widehat{p} \frac{1}{2m(\widehat{y})} \widehat{p} - \frac{\widehat{p}^2}{2m_\infty} + V(\widehat{y}) \end{pmatrix},\quad (91)$$

and is finally found in an outgoing Floquet state,

$$|\phi_{\text{out}}^{\text{AG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2k}} e^{+ikx} \begin{pmatrix} 1 \\ 0 \end{pmatrix}.\quad (92)$$

The other outgoing Floquet channel,

$$|\phi_{\text{out}}^{\text{AG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2K}} e^{+iKx} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \frac{\hbar^2K^2}{2m_\infty} = \frac{\hbar^2k^2}{2m_\infty} - \hbar\omega,\quad (93)$$

is closed in the studied range of electron impact energies, and can thus be ignored as we did already in Sec. IV A. The studied transmission process is completely characterized by the corresponding transmission coefficients, which are determined by the Lippmann-Schwinger formula

$$T_{\text{AG}}(E) = 1 - 2\pi i \langle\langle \phi_{\text{out}}^{\text{AG}} | \widehat{\mathcal{V}}_{\text{AG}} + \widehat{\mathcal{V}}_{\text{AG}} \frac{1}{E - \widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}}} \widehat{\mathcal{V}}_{\text{AG}} | \phi_{\text{in}}^{\text{AG}} \rangle\rangle.\quad (94)$$

Recall that $E = \frac{\hbar^2k^2}{2m_\infty}$ represents here of course the (quasi)energy of the incoming electron state (90). No singularity is encountered in $(E - \widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}})^{-1}$, since all the (resonance and continuum) eigenvalues of the non-Hermitian Hamilto-

where now

$$\widehat{\mathcal{Q}}\widehat{\mathcal{M}} = \widehat{\mathcal{Q}}\widehat{\mathcal{M}} \cos(\omega t), \quad \widehat{\mathcal{Q}}\widehat{\mathcal{M}} = \frac{\hbar^2}{4} \left(\frac{[m^{-1}(\widehat{y})]''}{m(\widehat{y})} \right)' \frac{q\alpha}{\omega}.\quad (86)$$

The second line of (85) neglects again all the terms of order higher than $O(\varepsilon_0)$, consistent with what is done in Sec. IV A.

Within the single-photon approximation, the above Hamiltonian $\widehat{\mathcal{H}}_{\text{AG}}$ of Eq. (85) can be converted into the following block matrix appearance:

Stated once again, the asymptotic AG Floquet Hamiltonian $\widehat{\mathcal{H}}_{\text{AG}}^{0,\text{NH}}$ of Eq. (89) is diagonal, and thus substantially simpler than its MG counterpart $\widehat{\mathcal{H}}_{\text{MG}}^{0,\text{NH}}$ [obtainable by changing \widehat{P} into \widehat{P}_f in Eq. (72)], meaning that the subsequent formulation of scattering theory is correspondingly more straightforward in AG compared to MG, due to the fact that an eigenvalue problem of $\widehat{\mathcal{H}}_{\text{AG}}^{0,\text{NH}}$ is resolvable trivially.

Our interest consists in studying the transmission phenomena, where an incoming electron prepared in a given asymptotic Floquet state,

$$|\phi_{\text{in}}^{\text{AG}}\rangle = \sqrt{\frac{m_\infty}{2\pi\hbar^2k}} e^{+ikx} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (k > 0)\quad (90)$$

(and carrying momentum $\hbar k$), is affected by an interaction

nian $\widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$ possess a negative imaginary part. Moreover, ECS does not affect the wave functions $|\phi_{\text{in,out}}^{\text{AG}}\rangle$ in the interaction region, and the situation is again similar as in Sec. IV A. Formulas (94), (87), and (91) lend themselves well to practical numerical calculations of $T_{\text{AG}}(E)$. Computational details will be given in Sec. IV C.

C. Numerical calculations and results

Our numerical calculations begin with solving the eigenvalue problems of the full Floquet Hamiltonians $\widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}}$ [Eq. (71)] and $\widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$ [Eq. (87)]. For this purpose we represent $\widehat{\mathcal{H}}_{\text{MG}}^{\text{NH}}$ and $\widehat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$ as matrices, using the sinc basis set

$$S_n(x) = \frac{1}{\sqrt{\Delta}} \text{sinc} \left[\pi \left(\frac{x}{\Delta} - n \right) \right] = \frac{\sqrt{\Delta}}{2} \int_{-\frac{1}{\Delta}}^{+\frac{1}{\Delta}} e^{+i\pi(x-n\Delta)v} dv.\quad (95)$$

Here, $\Delta > 0$ is a fixed numerical parameter, and $-n_{\text{max}} \leq n \leq +n_{\text{max}}$ with n_{max} being some cutoff value. Clearly, one has

$$S_n(x) \rightarrow \sqrt{\Delta} \delta(x - n\Delta) \quad (\Delta \rightarrow +0).\quad (96)$$

Hence $S_n(x)$ can be viewed as a smoothed Dirac delta function centered at $x = n\Delta$. The usual orthonormality relations apply,

$${}_x\langle S_n | S_{n'} \rangle_x = \int_{-\infty}^{+\infty} S_n(x) S_{n'}(x) dx = \delta_{nn'}. \quad (97)$$

Let \hat{Q} be any operator acting in the space of x -dependent functions. Its matrix representation over the above-discussed sinc basis set can be, to a good approximation, constructed as follows:

$$\begin{aligned} {}_x\langle S_n | \hat{Q} | S_{n'} \rangle_x &= \int_{-\infty}^{+\infty} S_n(x) (\hat{Q} S_{n'})(x) dx \\ &\doteq \sqrt{\Delta} \int_{-\infty}^{+\infty} \delta(x - n\Delta) (\hat{Q} S_{n'})(x) dx \\ &= \sqrt{\Delta} (\hat{Q} S_{n'})(n\Delta). \end{aligned} \quad (98)$$

We have taken advantage here of the above property (96). In particular, we have

$${}_x\langle S_n | \hat{P}_f | S_{n'} \rangle_x = \begin{cases} e^{-i\theta} {}_x\langle S_n | \hat{P} | S_{n'} \rangle_x, & |n|\Delta > x_0, \\ {}_x\langle S_n | \hat{P} | S_{n'} \rangle_x, & |n|\Delta \leq x_0. \end{cases} \quad (99)$$

Similarly of course for the case of ${}_y\langle S_n | \hat{P}_f | S_{n'} \rangle_y$. The just presented computational approach links the used sinc basis set to the discrete variable representation (DVR) formalism, and this point is elaborated explicitly in Ref. [17].

Prescriptions (98) and (99) enable us to build up the matrix representations of $\hat{\mathcal{H}}_{\text{MG}}^{\text{NH}}$ and $\hat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$ in a very efficient manner, since no numerical integration is involved. Subsequent numerical diagonalization of the just mentioned matrices provides the spectral representations of $\hat{\mathcal{H}}_{\text{MG}}^{\text{NH}}$ and $\hat{\mathcal{H}}_{\text{AG}}^{\text{NH}}$. The associated resolvents $(E - \hat{\mathcal{H}}_{\text{MG}}^{\text{NH}})^{-1}$ and $(E - \hat{\mathcal{H}}_{\text{AG}}^{\text{NH}})^{-1}$ are then also immediately accessible in this way.

Having in hand the resolvents $(E - \hat{\mathcal{H}}_{\text{MG}}^{\text{NH}})^{-1}$ and $(E - \hat{\mathcal{H}}_{\text{AG}}^{\text{NH}})^{-1}$, we are ready to tackle the transmission coefficients $T_{\text{MG}}(E)$ [Eq. (83)] and $T_{\text{AG}}(E)$ [Eq. (94)]. The interaction matrices \hat{V}_{MG} and \hat{V}_{AG} are again represented in the sinc basis set, exactly as already described above. A similar approach is of course implemented also in the case of the pertinent incoming/outgoing states. One has

$${}_x\langle S_n | |\phi_{\text{in/out}}\rangle \rangle = \sqrt{\Delta} |\phi_{\text{in/out}}\rangle \Big|_{x=n\Delta}. \quad (100)$$

The sought transmission coefficients $T_{\text{MG}}(E)$ [Eq. (83)] and $T_{\text{AG}}(E)$ [Eq. (94)] can be then evaluated straightforwardly for any value of the incoming electronic energy E .

In all our calculations, we have used atomic units ($c = 137.036$ a.u.). The potential function takes the form

$$V(x) = (0.025x^2 - 0.8)e^{-0.005x^2} \quad (101)$$

(see the upper panel of Fig. 1 in Sec. II). Almost the same kind of potential has been employed in our previous work [2].⁸ The ECS parameters have been chosen to be $x_0 = 150$ a.u. and $\theta = 0.5$. Parameter Δ of the sinc basis set was set to 1, and $n_{\text{max}} = 200$. Tests revealed that such numerical specifications are fully sufficient to provide satisfactory convergence for $T_{\text{MG}}(E)$ and $T_{\text{AG}}(E)$ along the entire studied energy range.

⁸Equation (101) sets $V(x) = v(x/\sqrt{2})$, where $v(x)$ is the potential of Ref. [2].

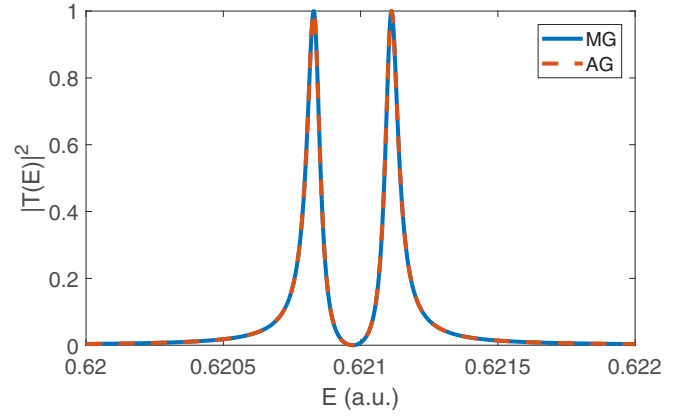


FIG. 3. Numerical illustration of the physical equivalence between the MG and AG Hamiltonians for the case when the electron mass is spatially independent. The transmission probability $|T(E)|^2$ is plotted here as a function of energy E of the incoming electron. One can see immediately that $|T_{\text{MG}}(E)|^2 = |T_{\text{AG}}(E)|^2$. We also point out that the just shown transmission dip profile arises due to the formation of an exceptional point [2].

As an additional check of convergence of our numerical results, we have also run analogous Floquet-based calculations of $T_{\text{MG}}(E)$ and $T_{\text{AG}}(E)$ reaching beyond the single-photon approximation. Namely, we have allowed for multiphoton dressing (by up to three photons). The obtained numerical outcomes (corresponding both to Figs. 1 and 2 from Sec. II C, and to Fig. 3 shown below) always turned out to be completely identical to their single-photon counterparts.

As our preliminary test calculation, we choose to investigate first a similar system as in Ref. [2]. This means that the electron mass is for now spatially independent, $m(x) = 0.05$ a.u. Recall that the computations of Ref. [2] have been done within the AG. The purpose of the just discussed preliminary calculation is thus to explicitly check an equivalence between the AG and MG modes of description. The pertinent laser field parameters are $\omega = 0.9189306021396$ a.u. and $\varepsilon_0 = 8.625863370106809 \times 10^{-5}$ a.u., such that the so-called exceptional point is formed [2].⁹ Our obtained results are plotted in Fig. 3. One can verify immediately that the agreement between our AG and MG calculations is excellent.

Our subsequent numerical illustrations are intended to explore the main topic of the present paper, namely, the effects of spatially dependent electron mass. The corresponding calculations have already been previewed in Sec. II C (see again Figs. 1 and 2). We shall thus only supplement here additional comments, and also details regarding the pertinent system parameters. Namely, the middle panel of Fig. 1 depicts the mass function $m(x) = 0.05V(x) + 0.05$ a.u., and similarly the upper panel of Fig. 2 shows the mass function $m(x) = 0.005V(x) + 0.05$ a.u..¹⁰ The laser field parameters are

⁹It is not the purpose of our present paper to discuss the exceptional points and their impact on transmission phenomena. The reader is relegated to Ref. [2] for the relevant information.

¹⁰We recall for clarity that such a choice of $m(x)$ is consistent with a physically motivated assumption that both $V(x)$ and $m(x)$

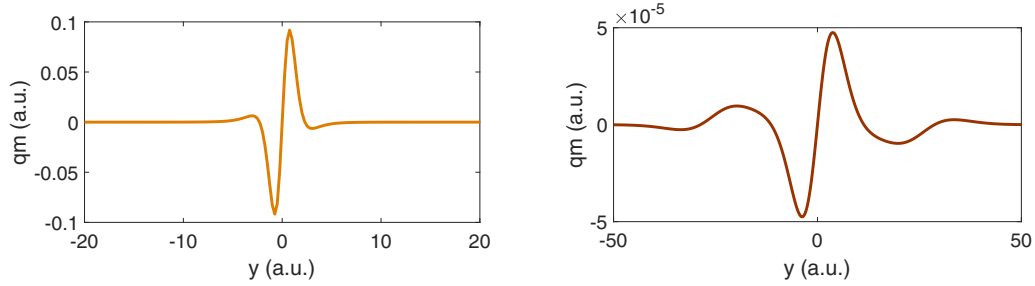


FIG. 4. The spatial profile of the extra quantum potential term \widehat{qm} of Eq. (86). Left panel: The system parameters of Fig. 1. Right panel: The system parameters of Fig. 2. One may observe that \widehat{qm} is by more than three orders of magnitude smaller on the right panel compared to the left panel. Also, the profile of \widehat{qm} is more smooth on the right panel.

follows: $\varepsilon_0 = 5 \times 10^{-4}$ a.u. (both for Figs. 1 and 2), $\omega = 1.3584$ a.u. (Fig. 1), and $\omega = 0.9391$ a.u. (Fig. 2). In both arrangements (both for Figs. 1 and 2), the associated value of $\hbar\omega$ is equal to the excitation energy between the (single) bound state and the lowest-lying resonance state supported by $V(x)$ and $m(x)$. In fact, the just given laser parameters are rather close to the exceptional point condition of Ref. [2], both for Figs. 1 and 2. It comes thus as no surprise that the calculated transmission profiles exhibit a dip. A more important insight (at least in the context of the present paper) consists in the fact that the calculated transmission probabilities $|T_{MG}(E)|^2$ and $|T_{AG}(E)|^2$ mutually agree both in Figs. 1 and 2, as long as the extra AG quantum term \widehat{QM} of Eqs. (68) or (86) is accounted for. An inclusion of \widehat{QM} turns out to be crucial in Fig. 1, whereas in Fig. 2 one may neglect \widehat{QM} to a reasonable approximation (this is not unexpected, since the spatial dependence of $m(x)$ is ten times less pronounced here than in the arrangement of Fig. 1). A more explicit insight into the nature of \widehat{QM} is provided by Fig. 4.

Even after including \widehat{QM} , there remains a tiny yet detectable difference between the MG and AG results, both in Figs. 1 and 2. This difference is most likely attributed to the weak-field approximation contained inherently in the AG Hamiltonian $\hat{H}_{AG}(t)$ of Eq. (67).

V. CONCLUDING REMARKS

In summary, we have established, in a thorough and systematic fashion, the concept of AG representation for a laser-driven nonrelativistic particle in the highly nontrivial and intriguing case of a position-dependent mass. Namely, in Sec. III A we have derived the classical AG Hamiltonian $H_{AG}(t)$ under the most general conditions, even without imposing the dipole approximation. It was shown that the resulting $H_{AG}(t)$ [given by Eq. (32)] possesses an unexpected structure arising solely just due to the spatial dependence of the mass. The construction of $H_{AG}(t)$ relies upon the generalized quiver amplitude $\mathbf{F}(t, y)$, which is defined as a unique

are determined by the local composition of the semiconductor material inside which the electron is set to move. Note also that the asymptotic region of $x \rightarrow \pm\infty$ corresponds to a constant (spatially homogeneous) semiconductor. This is why $m(x \rightarrow \pm\infty)$ approaches a constant value of 0.05 a.u. which still differs from the usual mass of an electron in free space.

solution of an initial value problem (30) and (31). Subsequently, we have dealt with the canonical quantization of the problem. Since an explicit construction of the AG Hamiltonian operator $\hat{H}_{AG}(t)$ does not seem to be easily tractable in its full generality, we have decided to restrict ourselves just to the regime of a weak laser intensity. The adequate weak-field AG Hamiltonian $\hat{H}_{AG}(t)$ was then derived in Sec. III B [Eq. (67)], where also its purely quantum mechanical component \widehat{QM} was explicitly written down [Eq. (68)]. Our theoretical findings have been illustrated numerically in Sec. IV, on a physically relevant phenomenon of resonance transmission of a monochromatically laser-driven electron through a model semiconductor nanostructure. Analogous MG calculations have been performed for the sake of comparison and reference. We have verified numerically the physical equivalence between the MG and the derived AG representation for our studied system. Importantly, we have demonstrated that the extra quantum mechanical contribution \widehat{QM} [of Eq. (68)] to $\hat{H}_{AG}(t)$ [Eq. (67)] often affects crucially the resulting profile of the electron transmission probability, which is a valuable physical insight *per se*.

We hope that our work can motivate further studies of the laser-induced dynamics of charged particles whose effective mass is spatially dependent. Note that the formalism presented here should be generalizable rather straightforwardly to a system of N mutually interacting particles (electrons).¹¹ Additional research may be aimed at the following directions: (a) finding the quantum mechanical AG Hamiltonian $\hat{H}_{AG}(t)$ appropriate in the moderate or strong field regimes, which can be possibly accomplished by employing the semiclassical \hbar -expansion technique mentioned at the end of Sec. III A; (b) looking for a physical interpretation and/or fingerprints of the AG quantum term \widehat{QM} [of Eq. (68)]; and (c) working out an adequate Hamiltonian in the length gauge.

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¹¹On the other hand, actual numerical computations would be of course much more demanding when it comes to a correlated N -electron system.

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