Relativistic treatment of harmonics from impurity systems in quantum wires

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Within a one-particle approximation of the Dirac equation we investigate a defect system in a quantum wire. We demonstrate that by minimally coupling a laser field of frequency ω to such an impurity system, one may generate harmonics of multiples of the incoming frequency. In a double defect system one may use the distance between the defects in order to tune the cutoff frequency.

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I. INTRODUCTION

Since the early 1990s, the generation of high-order harmonics of a strong, low-frequency laser field has attracted a lot of attention in the atomic physics community; see, e.g., Refs. 1 and 2 for a fairly recent review. Indeed, high-harmonic generation has opened a wide range of possibilities for obtaining high-frequency coherent sources, converting infrared input radiation of frequency ω into light in the extreme ultraviolet regime whose frequencies are multiples of ω (even up to order $\sim$1000; see, e.g., Ref. 2 for a recent review).

In gases, composed of atoms or small molecules, this phenomenon is well understood and, to some extent, even controllable in the sense that the frequency of the highest harmonic, the so-called ''cutoff,'' can be tuned as well as the intensities of particular groups of harmonics. In more complex systems, however, as for instance solids, or larger molecules, high-harmonic generation is still an open problem. This is due to the fact that, until a few years ago, such systems were expected not to survive the strong laser fields involved. However, nowadays, with the advent of ultrashort pulses, there exist solid-state materials whose damage threshold is beyond the required intensities of 10^{14} W/cm^2.[3] As a direct consequence, there is an increasing interest in such materials as potential sources for high harmonics. In fact, several groups are currently investigating this phenomenon in systems such as thin crystals,[4,5] carbon nanotubes,[6] or organic molecules.[7,8]

Prototype solid-state devices are quantum wires, which nowadays do not only serve as a theoretical test ground, but may even be studied experimentally, e.g., Ref. 9. With regard to the previously outlined problematic it is of great interest to investigate how such devices interact with laser light. In particular, the question of whether such systems are suitable high-harmonic sources has not been dealt with up to now. This is the central question which we shall be answering positively in this manuscript.

A useful particularity of quantum wires is that they are the physical realization of models involving only one spatial dimension. Considering theories in one space dimension has the further virtue that it allowed for the development of various powerful nonperturbative techniques, which exploit the integrability of the models. For instance, one may compute the conductance of quantum wires in this fashion, see, e.g., Ref. 10, and references therein. This also suggests that an exact relativistic treatment of the electrons in the wire in the presence of the laser field is possible. Therefore such a treatment constitutes an advantage over most approaches adopted in the literature, in the context of atoms in strong laser fields, which involve a series of approximations. The first, and most general approximation performed in this context is that a proper field-theoretical treatment is usually not taken into account. Furthermore, when dealing with a relativistic situation, the Dirac equation is solved mostly by numerical methods, which by themselves involve a series of approximation and exhibit a good convergence only for high-frequency fields.[11] Further approximations include the expansion[12] of the Dirac equation for the weakly relativistic case, the solution of the Klein-Gordon equation[13,14] or of the relativistic Schrödinger equation, or purely classical treatments.[15] For some recent general reviews see, e.g., Ref. 16.

In this paper, we solve the Dirac equation for an electron in a quantum wire subject to an external laser field, including a single and multiple defects. We investigate in various different regimes the radiation emitted by an electron in this system in connection with the transmission at the defects and demonstrate that the generation of harmonics is possible in such systems.

II. DEFECT SYSTEMS IN LASER FIELDS

Since the work of Weyl,[17] one knows that matter may be coupled to light by means of a local gauge transformation, which reflects itself in the usual minimal coupling prescription, i.e., $\partial_\mu \rightarrow \partial_\mu - ieA_\mu$, with A_μ being the vector gauge potential. For a free Fermion with mass m this yields to the Lagrangian density

$$\mathcal{L}_A = \overline{\psi}(i\gamma^\mu \partial_\mu - m + e\gamma^\mu A_\mu)\psi. \tag{1}$$

We adopt here relativistic units $1=c=\hbar=m\approx e^2 137$ as mostly used in the particle physics context rather than atomic units $1=e=\hbar=m\approx c/137$ useful in atomic physics. As common conventions we abbreviated here $\overline{\psi}=\psi^\dagger\gamma^0$ and use the following realization for the gamma matrices:

$$\gamma^0=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \gamma^1=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},\quad \gamma^5=\gamma^0\gamma^1. \tag{2}$$

In the absence of the laser field the equations of motion for the free Fermion may be solved by the well-known Fourier decomposition,

$$\psi_j^f(x,t)=\int \frac{d\theta}{\sqrt{4\pi}}[a_j(\theta)u_j(\theta)e^{-i\vec{p}_j\cdot\vec{x}}+a_j^\dagger(\theta)v_j(\theta)e^{i\vec{p}_j\cdot\vec{x}}]. \tag{3}$$

We parametrize the momentum as common through the rapidity θ by $p_j^0=m_j\cosh\theta$, $p_j^1=m_j\ \sinh\theta$ and denote the antiparticle (positron) of the Fermion (electron) j by $\overline{j}$. For the Weyl spinors we employ the normalization

$$u_j(\theta)=-i\gamma^5 v_j(\theta)=\sqrt{\frac{m_j}{2}}\begin{pmatrix}e^{-\theta/2}\\ e^{\theta/2}\end{pmatrix}, \tag{4}$$

and the creation and annihilation operators $a_i(\theta)$, $a_i^\dagger(\theta)$ for a particle with rapidity θ obey the usual Fermionic anticommutation relations $\{a_i(\theta_1),a_j(\theta_2)\}=0$, $\{a_i(\theta_1),a_j^\dagger(\theta_2)\}=2\pi\delta_{ij}\delta(\theta_1-\theta_2)$. When the laser field is switched on, we can solve the equation of motion associated to Eq. (1),

$$(i\gamma^\mu\partial_\mu-m+e\gamma^\mu A_\mu)\psi=0, \tag{5}$$

by a Gordon-Volkov type solution,[18]

$$\psi_j^A(x,t)=\exp\left[ie\int^x dsA_1(s,t)\right]\psi_j^f(x,t), \tag{6}$$

$$=\exp\left[ie\int^t dsA_0(x,s)\right]\psi_j^f(x,t). \tag{7}$$

Using now a linearly polarized laser field along the direction of the wire, the vector potential can typically be taken in the dipole approximation to be a superposition of monochromatic light with frequency ω, i.e.,

$$A(t):=A_1(t)=\frac{1}{x}\int_0^t dsA_0(s) \tag{8}$$

$$=-\frac{1}{2}\int_0^t dsE(s)=-\frac{E_0}{2}\int_0^t dsf(s)\cos(\omega s) \tag{9}$$

with $f(t)$ being an arbitrary enveloping function equal to zero for $t<0$ and $t>\tau$, such that τ denotes the pulse length. In the following we will always take $f(t)=\Theta(t)\Theta(\tau-t)$, with $\Theta(x)$ being the Heaviside unit step function. The second equality in Eq. (8), $A_0(x,t)=x\dot{A}(t)$, follows from the fact that we have to solve Eqs. (6) and (7).

One comment is due with regard to the validity of the dipole approximation in this context. It consists usually in neglecting the spatial dependence of the laser field, which is justified when $x\omega<c=1$, where x is a representative scale of the problem considered. In the context of atomic physics this is typically the Bohr radius. In the problem investigated here, this approximation has to hold over the full spatial range in which the Fermion follows the electric field. We can estimate this classically, in which case the maximal amplitude is eE_0/ω^2 and therefore the following constraint has to hold,

$$\left(\frac{eE_0}{\omega}\right)^2=4U_p<1, \tag{10}$$

for the dipole approximation to be valid. Due to the fact that x is a function of ω, we have now a lower bound on the frequency rather than an upper one as is more common in the context of atomic physics. We have also introduced here the ponderomotive energy U_p for monochromatic light, that is the average kinetic energy transferred from the laser field to the electron.

The solutions to the equations of motion of the free system and the one which includes the laser field are then related by a factor similar to the gauge transformation from the length to the velocity gauge

$$\psi_j^A(x,t)=\exp[ixeA(t)]\psi_j^f(x). \tag{11}$$

In an analogous fashion one may use the same minimal coupling procedure also to couple in addition the laser field to the defect. One has to invoke the equation of motion in order to carry this out, since as in Ref. 10, we assume here also that the defect is linear in the fields $\overline{\psi}$ and ψ. The Lagrangian density for a complex free Fermion ψ with ℓ defects $\mathcal{D}^\alpha(\overline{\psi},\psi,A_\mu)$ of type α at the position x_n subjected to a laser field then reads

$$\mathcal{L}_{AD}=\mathcal{L}_A+\sum_{n=1}^{\ell}\mathcal{D}^{\alpha_n}(\overline{\psi},\psi,A_\mu)\delta(x_n). \tag{12}$$

Considering for simplicity first the case of a single defect situated at $x=0$, the solution to the equation of motion resulting from Eq. (12) is taken to be of the form

$$\psi_j^A(x,t)=\Theta(x)\psi_{j,+}^A(x,t)+\Theta(-x)\psi_{j,-}^A(x,t). \tag{13}$$

This means we distinguish here by notation the solutions (11) on the left and right of the defect, $\psi_{j,-}^A(x,t)$ and $\psi_{j,+}^A(x,t)$, respectively. This is also reflected in the corresponding creation and annihilation operators $a_{j,+}(\theta)$, $a_{j,-}(\theta)$, etc. One may then proceed according to standard potential scattering theory and notes that these functions are not independent of each other. Substitution of Eq. (13) into the equation of motion yields the constraints

$$i\gamma^1[\psi_{j,+}^A(x,t)-\psi_{j,-}^A(x,t)]\Big|_{x=0}=\frac{\partial\mathcal{D}_{AD}(\overline{\psi},\psi,A_\mu)}{\partial\overline{\psi}_j^A(x,t)}\Big|_{x=0}. \tag{14}$$

These restrictions (14) serve to determine the transmission and reflection amplitudes. The extension to multiple defects, that is having equations of the type (14) for each defect situated at position $x=x_n$, follows in an analogous straightforward manner.

A. Transmission and reflection amplitudes

Substituting the Fourier decomposition (3), together with the free Fermion solution minimally coupled to a laser field

(11) into the constraint (14), one can determine the reflection and transmission amplitudes from the left to the right, R and T, respectively. They are defined in an obvious manner as

$$a_{j,-}(\theta)=R_j(\theta)a_{j,-}(-\theta)+T_j(\theta)a_{j,+}(\theta). \tag{15}$$

When parity invariance is broken, the corresponding amplitudes from the right to the left do not have to be identical and are defined as

$$a_{j,+}(-\theta)=\tilde{T}_j(\theta)a_{j,-}(-\theta)+\tilde{R}_j(\theta)a_{j,+}(\theta). \tag{16}$$

In this way the laser field parameters E_0 and ω will be quantities on which the R's and T's depend upon at a particular time t. When iterating these equations one obtains the corresponding expressions for multiple defect systems, e.g., placing for instance the defect $\mathcal{D}^\alpha$ left from $\mathcal{D}^\beta$ one obtains the well-known expressions

$$T_i^{\alpha\beta}(\theta)=\frac{T_i^\alpha(\theta)T_i^\beta(\theta)}{1-R_i^\beta(\theta)\tilde{R}_i^\alpha(\theta)}, \tag{17}$$

$$R_i^{\alpha\beta}(\theta)=R_i^\alpha(\theta)+\frac{R_i^\beta(\theta)T_i^\alpha(\theta)\tilde{T}_i^\alpha(\theta)}{1-R_i^\beta(\theta)\tilde{R}_i^\alpha(\theta)}. \tag{18}$$

From our previous comment on the validity of the dipole approximation it is clear that the distance between the two defects introduces a new scale in the system, which has to be constrained as $y<\omega^{-1}$. In addition, to justify that the multiple defect system can be treated effectively as a single one requires that the sum of the y's is much smaller than the length of the wire. Similar expressions, which we will not need in what follows, hold for the parity reversed situation and for more defects; see, e.g., Ref. 10 and references therein.

In addition with regard to the application of high harmonic generation, we shall be interested in the spectrum of frequencies which are filtered out by the defect while the laser pulse is nonzero. The Fourier transforms of the reflection and transmission probabilities provide exactly this information:

$$\mathcal{T}(\Omega,\theta,E_0,\omega,\tau)=\frac{1}{\tau}\int_0^\tau dt|T(\theta,E_0,\omega,t)|^2\cos(\Omega t), \tag{19}$$

$$\mathcal{R}(\Omega,\theta,E_0,\omega,\tau)=\frac{1}{\tau}\int_0^\tau dt|R(\theta,E_0,\omega,t)|^2\cos(\Omega t). \tag{20}$$

When parity is preserved for the reflection amplitudes, we have $|T|^2+|R|^2=1$, and it suffices to consider $\mathcal{T}$ in the following.

1. Type-I defects

Taking the laser field in form of monochromatic light in the dipole approximation (9), we may naturally assume that the transmission probability for some particular defects can be expanded as

$$|T_I(\theta,U_p,\omega,t)|^2=\sum_{k=0}^\infty t_{2k}(\theta)(4U_p)^k\sin^{2k}(\omega t). \tag{21}$$

We shall refer to defects which admit such an expansion as "type-I defects." Assuming that the coefficients $t_{2k}(\theta)$ become at most 1, we have to restrict our attention to the regime $4U_p<1$ in order for this expansion to be meaningful for all t. Note that this is no further limitation, since it is precisely the same constraint as already encountered for the validity of the dipole approximation (10). The first coefficient is always the transmission probability for vanishing laser field, that is $t_0(\theta)=|T(\theta,E_0=0)|^2$. The functional dependence of Eq. (21) will turn out to hold for various explicit defects considered below. Based on this equation, we compute for such type of defect

$$\mathcal{T}_I(\Omega,\theta,U_p,\omega,\tau)=\sum_{k=0}^\infty \frac{(2k)!(U_p)^k\sin(\tau\Omega)t_{2k}(\theta)}{\tau\Omega\prod_{l=1}^k[l^2-(\Omega/2\omega)^2]}. \tag{22}$$

It is clear from this expression that type-I defects will preferably let even multiples of the basic frequency ω pass, whose amplitudes will depend on the coefficients $t_{2k}(\theta)$. When we choose the pulse length to be integer cycles, i.e., $\tau=2\pi n/\omega=nT$ for $n\in\mathbb{Z}$, the expression in Eq. (22) reduces even further. The values at even multiples of the basic frequency are simply

$$\mathcal{T}_I(2n\omega,\theta,U_p)=(-1)^n\sum_{k=0}^\infty t_{2k}(\theta)(U_p)^k\binom{2k}{k-n}, \tag{23}$$

which becomes independent of the pulse length τ. Notice also that the dependence on E_0 and ω occurs in the combination of the ponderomotive energy U_p. Further statements require the precise form of the coefficients $t_{2k}(\theta)$ and can only be made with regard to a more concrete form of the defect.

2. Type-II defects

Clearly, not all defects are of the form (21) and we have to consider also expansions of the type

$$|T_{II}(\theta,E_0/e,\omega,t)|^2=\sum_{k,p=0}^\infty t_{2k}^p(\theta)\frac{E_0^{2k+p}}{\omega^{2k}}\cos^p(\omega t)\sin^{2k}(\omega t). \tag{24}$$

We shall refer to defects which admit such an expansion as "type-II defects." In this case we obtain

$$\mathcal{T}_{II}(\Omega,\theta,E_0/e,\omega,\tau)=\sum_{k,p=0}^{\infty}\sum_{l=0}^{p}\binom{p}{l}\frac{\Omega\sin(\tau\Omega)}{(-1)^{l+1}\tau\omega^{2+2k}}\times\left(\frac{(2k+2l)!t_{2k}^{2p}(\theta)}{\prod_{q=0}^{k+l}\left[(2q)^2-\left(\frac{\Omega}{\omega}\right)^2\right]}+\frac{(2k+2l)!t_{2k}^{2p+1}(\theta)E_0}{\prod_{q=1}^{k+l+1}\left[(2q-1)^2-\left(\frac{\Omega}{\omega}\right)^2\right]}\right)E_0^{2k+2p}. \tag{25}$$

We observe from this expression that type-II defects will filter out all multiples of ω. For the pulse being once again of integer cycle length, this reduces to

$$\mathcal{T}_{II}(2n\omega,\theta,U_p,E_0)=\sum_{k,p=0}^{\infty}\sum_{l=0}^{p}\binom{2k+2l}{k+l-n}\times(-1)^{l+n}\frac{t_{2k}^{2p}(\theta)}{2^{2l-2p}}(U_p)^{k+p}E_0^{2p}\binom{p}{l} \tag{26}$$

and

$$\mathcal{T}_{II}((2n-1)\omega,\theta,E_0/e)=\sum_{k,p=0}^{\infty}\sum_{l=0}^{p}(-1)^{l+n+1}\frac{t_{2k}^{2p+1}(\theta)}{2^{2l-2p+1}}\times(U_p)^{k+p}\binom{p}{l}\frac{(2k+2l)!(2n-1)E_0^{2p+1}}{(l+k-n+1)!(l+n+k)!} \tag{27}$$

which are again independent of τ. We observe that in this case we cannot combine the E_0 and ω into a U_p. The analytical expressions presented in this section will not only serve as a benchmark for our analytical computation, but can be used in addition to extract various structural information as we see below.

B. One-particle approximation

In spite of the fact that we are dealing with a quantum field theory, it is known that a one-particle approximation to the Dirac equation is very useful and physically sensible when the external forces vary only slowly on a scale of a few Compton wavelengths; see e.g., Ref. 19. We may therefore define the spinor wave functions

$$\Psi_{j,u,\theta}(x,t):=\psi_j^A(x,t)\frac{|a_j^\dagger(\theta)\rangle}{\sqrt{2\pi^2p_j^0}}=\frac{e^{-i\vec{p}_j\cdot\vec{x}}}{\sqrt{2\pi p_j^0}}u_j(\theta), \tag{28}$$

$$\Psi_{j,v,\theta}(x,t)^\dagger:=\psi_j^A(x,t)^\dagger\frac{|a_j^\dagger(\theta)\rangle}{\sqrt{2\pi^2p_j^0}}=\frac{e^{-i\vec{p}_j\cdot\vec{x}}}{\sqrt{2\pi p_j^0}}v_j(\theta)^\dagger. \tag{29}$$

With the help of these functions we obtain then for the defect system

$$\mathbf{\Psi}_{i,u,\theta}^A(x,t):=\psi_i^A(x,t)\frac{|a_{i,-}^\dagger(\theta)\rangle}{\sqrt{2\pi^2p_i^0}}=\Theta(-x)[\Psi_{i,u,\theta}(x,t)+\Psi_{i,u,-\theta}(x,t)R_i^*(\theta)]+\Theta(x)T_i^*(\theta)\times[\Psi_{i,u,\theta}(x,t)+\Psi_{i,u,-\theta}(x,t)\tilde{R}_i^*(-\theta)] \tag{30}$$

and the same function with $u\to v$. Since this function resembles a free wave it cannot be normalized properly and we have to localize the wave in form of a wave packet by multiplying with an additional function, $\tilde{g}(p,t)$ in Eq. (3) and its counterpart $g(x,t)$ in Eq. (30), typically a Gaussian. Then for the function $\mathbf{\Phi}_{i,u,\theta}^A(x,t)=g(x,t)\mathbf{\Psi}_{i,u,\theta}^A(x,t)$, we can achieve that $\|\mathbf{\Phi}\|=1$.

III. HARMONIC GENERATION

As mentioned above, harmonic generation has attracted large attention in the atomic physics community in recent years. It is the nonlinear response of a dipole moment, in general atomic, to an external laser field. Here we want to investigate whether such responses also exist for defect systems. We carry out our treatment relativistically. The time-dependent dipole moment is given by

$$x_{j,u,\theta}(t)=\langle\mathbf{\Phi}_{j,u,\theta}^A(x,t)^\dagger x\mathbf{\Phi}_{j,u,\theta}^A(x,t)\rangle \tag{31}$$

such that the emission spectrum is the absolute value of the Fourier transform of the dipole moment

$$\mathcal{X}_{j,u,\theta}(\Omega)=\left|\int_0^\tau dt\,x_{j,u,\theta}(t)\exp i\Omega t\right|. \tag{32}$$

We localize now the wave packet in a region much smaller than the classical estimate for the maximal amplitude the electron will acquire when following the laser field. We achieve this with a Gaussian $g(x,t)=\exp(-x^2/\Delta)$, where $\Delta\ll eE_0/\omega^2$. Placing the defect at the origin and neglecting its extension, the computation of Eq. (31) with Eq. (30) then boils down to the evaluation of

$$x_{i,u,\theta}(t)=\int_{-\infty}^{0}\frac{x\left[1+|R_i(\theta)|^2+2\,\mathrm{Re}\dfrac{e^{2ix\sinh\theta}R_i(\theta)}{\cosh\theta}\right]}{2\pi e^{(2/\Delta)[x+eA(t)]^2}}dx+\int_0^\infty\times\frac{x|T_i(\theta)|^2\left[1+|R_i(\theta)|^2+2\,\mathrm{Re}\dfrac{e^{2ix\sinh\theta}R_i(\theta)^*}{\cosh\theta}\right]}{2\pi e^{(2/\Delta)[x+eA(t)]^2}}dx. \tag{33}$$

The expressions for the R's and T's depend of course on the form of the defect and further generic statements cannot be made at this point. We therefore turn to a concrete example.

IV. ENERGY OPERATOR DEFECT

Localizing sharply the energy operator $\varepsilon(x)=g\bar{\psi}\psi(x)$, with g being a coupling constant, yields a defect which has been studied extensively in the absence of a laser field. It should be noted that this is only a particular example and one may also consider other type of defects in a analogous fashion; see Ref. 10 and references therein. One of the virtues of this defect is that it is real, thus preserving parity invariance.

Coupling the vector potential minimally to this type of defect yields

$$\mathcal{D}_{AD}(\bar{\psi},\psi,A_\mu)=g\bar{\psi}(1+e/m\,\gamma^\mu A_\mu)\psi, \tag{34}$$

by invoking the equation of motion.

A. Transmission and reflection amplitudes

We are now interested in determining the reflection and transmission amplitudes associated to this defect by the potential scattering method as outlined in Sec. II A. Taking from now on $m=1$, we compute for the various reflection amplitudes

$$\begin{aligned}
&R_i(\theta,g,A/e,y)\\
&\quad=\tilde{R}_i(\theta,g,-A/e,-y)=R_{\bar{i}}(\theta,g,A/e,-y)\\
&\quad=\tilde{R}_{\bar{i}}(\theta,g,-A/e,y)\\
&\quad=\frac{[y\dot{A}-\cosh\theta]e^{-2iy\,\sinh\theta}}{[1-y\dot{A}\cosh\theta]-i\dfrac{g}{4}\left[\dfrac{4}{g^2}+1+A^2-y^2\dot{A}^2\right]\sinh\theta}.
\end{aligned} \tag{35}$$

We denoted the differentiation with respect to time by a dot. The transmission amplitudes turn out to be

$$\begin{aligned}
&T_i(\theta,g,A/e,y)\\
&\quad=\tilde{T}_i(\theta,g,-A/e,-y)=T_{\bar{i}}(\theta,g,-A/e,y)\\
&\quad=\tilde{T}_{\bar{i}}(\theta,g,A/e,-y)\\
&\quad=\frac{i\left[1-y^2\dot{A}^2+\left(A-\dfrac{2i}{g}\right)^2\right]\sinh\theta}{\dfrac{4}{g}[1-y\dot{A}\cosh\theta]-i\left[\dfrac{4}{g^2}+1+A^2-y^2\dot{A}^2\right]\sinh\theta}.
\end{aligned} \tag{36}$$

Locating the defect at $y=0$, the derivative of A does not appear anymore explicitly in Eqs. (35) and (36), such that it is clear that this defect is of type I and admits an expansion of the form Eq. (21). With the explicit expressions (35) and (36) at hand, we can determine all the coefficients $t_{2k}(\theta)$ in Eq. (21) analytically. For this purpose let us first bring the transmission amplitude into the more symmetric form,

$$|T_i(\theta,g,A/e)|^2=\frac{\tilde{a}_0(\theta,g)+a_2(\theta,g)A^2+a_4(\theta,g)A^4}{a_0(\theta,g)+a_2(\theta,g)A^2+a_4(\theta,g)A^4}, \tag{37}$$

with

$$a_0(\theta,g)=16g^2+(4+g^2)^2\sinh^2\theta, \tag{38}$$

$$\tilde{a}_0(\theta,g)=(g^2-4)^2\sinh^2\theta, \tag{39}$$

$$a_2(\theta,g)=2g^2(4+g^2)\sinh^2\theta, \tag{40}$$

$$a_4(\theta,g)=g^4\sinh^2\theta. \tag{41}$$

We can now expand $|T(\theta,g,A)|^2$ in powers of the field $A(t)$ and identify the coefficients $t_{2k}(\theta,g)$ in Eq. (21) thereafter. To achieve this we simply have to carry out the series expansion of the denominator in Eq. (37). The latter admits the following compact form:

$$\frac{1}{a_0(\theta,g)+a_2(\theta,g)A^2+a_4(\theta,g)A^4}=\sum_{k=0}^{\infty}c_{2k}(\theta,g)A^{2k},$$

with

$$c_0(\theta,g)=1/a_0(\theta,g)$$

and

$$c_{2k}(\theta,g)=-\frac{c_{2k-2}(\theta,g)a_2(\theta,g)+c_{2k-4}(\theta,g)a_4(\theta,g)}{a_0(\theta,g)},$$

for $k>0$. We understand here that all coefficients c_{2k} with $k<0$ are vanishing, such that from this formula all the coefficients c_{2k} may be computed recursively. Hence, by comparing with the series expansion (21), we find the following closed formula for the coefficients $t_{2k}(\theta,g)$:

$$t_{2k}(\theta,g)=[\tilde{a}_0(\theta,g)-a_0(\theta,g)]c_{2k}(\theta,g)\quad k>0. \tag{42}$$

The first coefficients then simply read

$$t_0(\theta,g)=\frac{\tilde{a}_0(\theta,g)}{a_0(\theta,g)}=|T(\theta,E_0=0)|^2, \tag{43}$$

$$t_2(\theta,g)=\frac{a_2(\theta,g)}{a_0(\theta,g)}[1-t_0(\theta,g)] \tag{44}$$

$$=\frac{8g^4(4+g^2)\sinh^2 2\theta}{(16g^2+(4+g^2)^2\sinh^2\theta)^2}, \tag{45}$$

$$t_4(\theta,g)=\left[\frac{a_4(\theta,g)}{a_2(\theta,g)}-\frac{a_2(\theta,g)}{a_0(\theta,g)}\right]t_2(\theta,g), \tag{46}$$

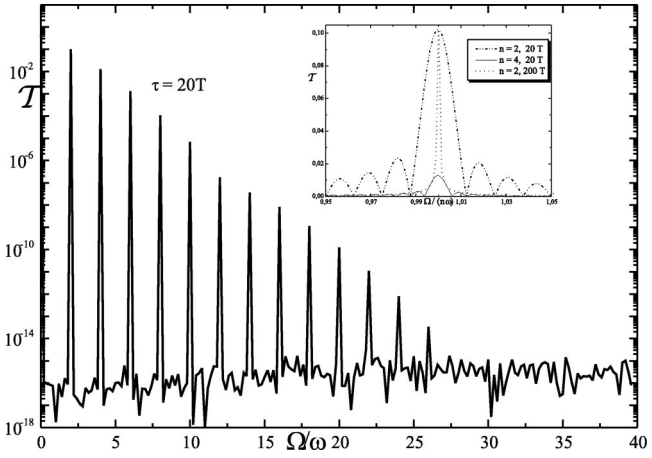

FIG. 1. Absolute value squared of the Fourier transform of the transmission probability for a single defect with $E_0=2.0$, $g=3.5$, $\theta=1.2$, $\omega=0.2$.

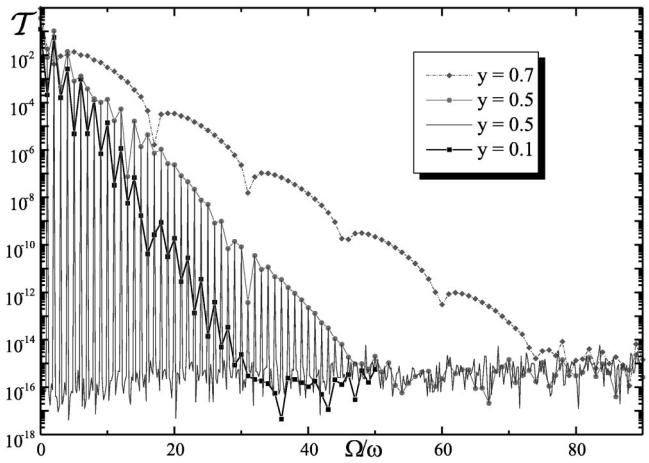

FIG. 2. Absolute value squared of the Fourier transform of the transmission probability for a double defect with $E_0=2.0$, $g=3.5$, $\theta=1.2$, $\omega=0.2$, and varying y.

and so on. It is now clear how to obtain also the higher terms analytically, but since they are rather cumbersome we do not report them here.

B. Harmonic generation

With the coefficients t_{2k}, we can compute the series (22) and (23) in principle to any desired order. For some concrete values of the laser and defect parameters the results of our evaluation are depicted in Fig. 1.

The main observation is that the defect acts as a filter selecting higher harmonics of even order of the laser frequency. Furthermore, from the zoom of the peak regions, we see that there are satellite peaks appearing near the main harmonics. They reduce their intensity when τ is increased, such that with longer pulse length the harmonics become more and more pronounced.

We also investigated that for different frequencies ω the general structure will not change. Increasing the field amplitude E_0, simply lifts up the whole plot without altering very much its overall structure. We support these findings in two alternative ways, either by computing directly Eq. (19) numerically or, more instructively, by evaluating the sums (22) and (23).

Let us now carry out a similar analysis for a double defect system. We place one of the defects at $x=0$ and the other at $x=y$. The distance emerges now as a new scale in the system and note from our comment on the validity of the dipole approximation that is restricted as $y<\omega^{-1}$. In addition y has to be much smaller than the total length of the wire. The double defect amplitudes are computed directly from Eqs. (17) and (18) with the expression for the single defect (35) and (36). Since now both A and $\dot{A}$ appear explicitly in the formulas for R's and T's, it is clear that the expansion of the double defect cannot be of type I, but it turns out to be of type II, i.e., of the form (24). Hence we will now expect that besides the even also the odd multiples of ω will be filtered out. This is confirmed by our explicit computations for two identical defects as depicted in Fig. 2.

Here we have only plotted a continuous spectrum for $y=0.5$, whereas for reasons of clarity, we only drew the enveloping function which connects the maxima of the harmonics for the remaining distances. We observe that now not only odd multiples of the frequency emerge in addition as harmonics, but also that we obtain much higher harmonics and the cutoff is shifted further to the ultraviolet. Furthermore, we see a periodic pattern in the enveloping function, which appears to be independent of y. Similar patterns were observed before in the literature, as for instance in the context of atomic physics described by a Klein-Gordon formalism (see Fig. 2 in Ref. 14).

With varying distance y the new structures can be modulated, i.e., we can control the intensity of certain peaks and also shift the cutoff. Clearly for a concrete application one would like the control mechanism to be as simple as possible and therefore it is interesting to investigate precisely how the emission amplitude and the cutoff behave as functions of y. Unfortunately, this function turns out to be not very simple as can be seen from Fig. 3, where we present our analysis for varying y and particular fixed harmonics. Nonetheless, there is a universal shape common to all harmonics of the same type. As expected from the analytical expressions the overall pattern for the odd and even harmonics differs. We confirm our previous observation, namely that for small values of the distance y, which corresponds to the limit of a single defect, there are no odd harmonics emerging.

Let us now come to the main point of our analysis and see how this structure is reflected in the harmonic spectrum. The result of the evaluation of Eq. (33) is depicted in Fig. 4.

We observe a very similar spectrum as we have already computed for the Fourier transform of the transmission amplitude, which is not entirely surprising with regard to the expression (33). The cutoff frequencies are essentially identical. From the comparison between $\mathcal{X}$ and the enveloping function for $\mathcal{T}$ we deduce that the term involving the transmission amplitude clearly dominates the spectrum.

Let us now turn to the computation of the emission spectrum for a double defect system coupled to a laser field. We depict the results of our analysis in Fig. 5.

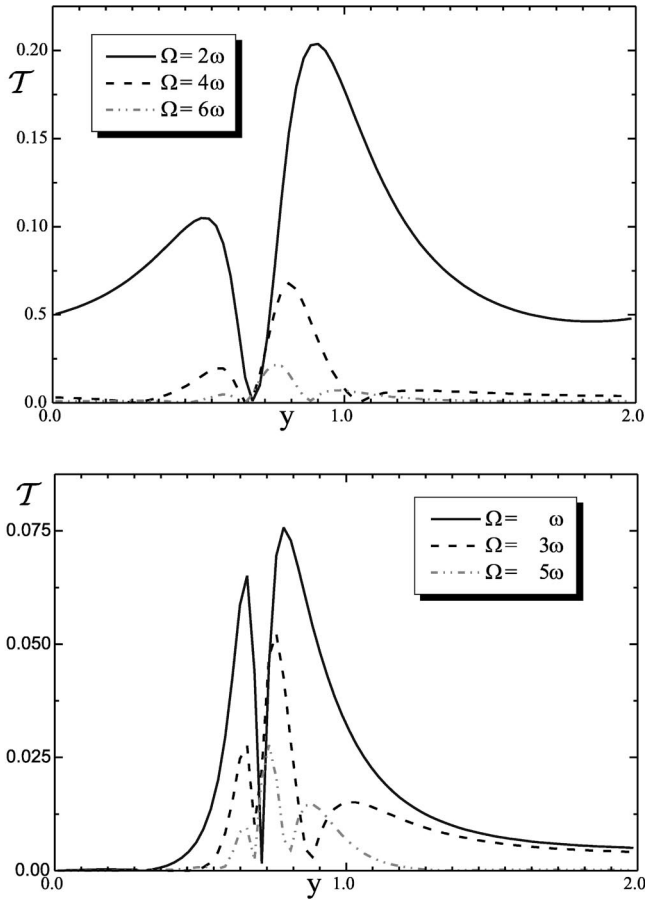

FIG. 3. Absolute value squared of the Fourier transform of the transmission probability for a double defect with $E_0=2.0$, $g=3.5$, $\theta=1.2$, for even and odd multiples of $\omega=0.2$ and varying y.

Once again, we observe a qualitatively similar behavior as for $\mathcal{T}$, in particular the occurrence of even and odd order harmonics. We remark that in our approach for larger values of y the normalization of the wave function becomes somewhat inaccurate and therefore the relative height in the intensities is not very precise. In principle this could be compensated, but for the conclusions we are trying to reach here that is not important. The important general deduction from these computations is of course that harmonics of higher order do emerge in the emission spectrum of a defect system.

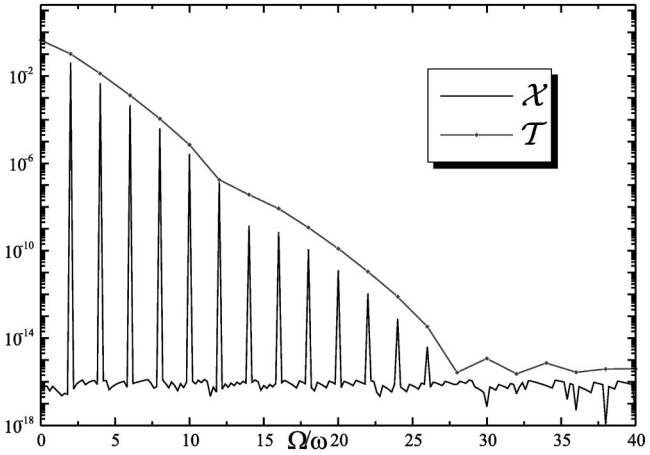

FIG. 4. Harmonic emission spectrum for a single defect with $E_0=2.0$, $g=3.5$, $\theta=1.2$, $\omega=0.2$, $\Delta=6$.

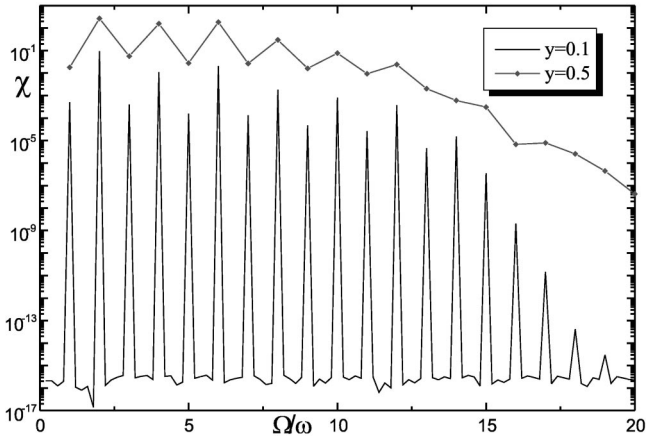

FIG. 5. Harmonic emission spectrum for a double defect with $E_0=2.0$, $g=3.5$, $\theta=1.2$, $\omega=0.2$, $\Delta=6$.

C. Relativistic versus nonrelativistic regime

In the previous sections we have been working in an intensity regime which is close to the damage threshold of a solid, according to the experimental observations in Ref. 3. This allowed us to see the maximum effect with regard to harmonic generation which at present might be visible from experiments. However, it is also interesting to investigate situations which are not experimentally feasible at present and of course lower intensity regimes.

In order to judge in which regime we are working and whether there are relativistic effects, let us carry out various limits. First of all we recall a standard estimation according to which the relativistic kinetic energy is close to the classical one when one is dealing with velocities $v^2 \ll 3/4c^2$. This is the same as saying that the kinetic energy is much smaller than the rest mass $E_{\mathrm{kin}} \ll m_0 c^2$. Making now a rough estimation for the system under consideration, we assume that the total kinetic energy is the one obtained from the laser field, i.e., the ponderomotive energy U_p. We also ignore for this estimation any sophisticated corrections, such as possible Doppler shifts in the frequency, etc. Then the nonrelativistic regime is characterized by the condition $U_p \ll 1$.

Based on our previous observation that $\mathcal{T}$ and $\mathcal{X}$ exhibit a very similar behavior, it will be sufficient here to study only the $\mathcal{T}$ in the different regimes, which will be easier than an investigation of the full emission spectrum (33). From our analytic expression (23), we see that for a type-I defect the quantity $\mathcal{T}_I$ becomes a function of U_p, such that the regime will be the same when we rescale simultaneously E_0 and ω. Accordingly we evaluate numerically the Fourier transform (19), or equivalently compare against our analytical expression (23), and depict our results in Fig. 6.

We observe that when passing more and more towards the relativistic regime the cutoff is increased. The other feature one recognizes is that the modulating structure in the envel-

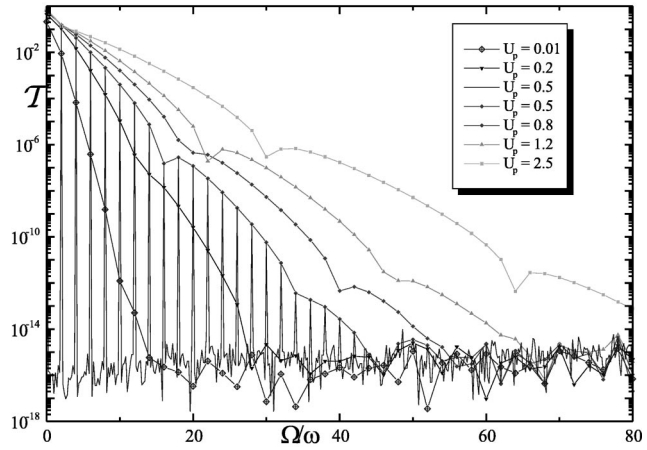

FIG. 6. Absolute value squared of the Fourier transform of the transmission probability for a single defect for various values of U_p with $g=3.5$, $\theta=1.2$.

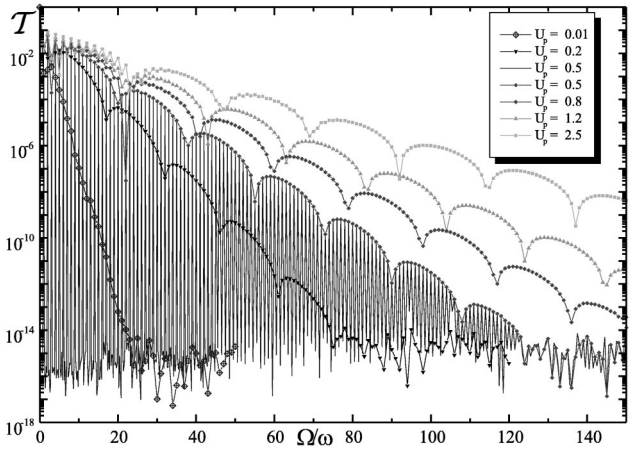

FIG. 7. Absolute value squared of the Fourier transform of the transmission probability for a double defect for varying values of E_0 with $g=3.5$, $\theta=1.2$, $\omega=0.2$.

oping function of the harmonics becomes more pronounced. One should also note, in regard to Eq. (10), that the multipole structures might become more and more important in the relativistic regime.

Let us now perform a similar computation for the double defect. From the expressions (26) and (27) we see that now $\mathcal{T}_{II}$ is not just a simple function of U_p and therefore even being in the same regime the behavior will be different when E_0 and ω are rescaled. We alter in that case the regimes by rescaling E_0 and keeping the frequency fixed. Our results are depicted in Fig. 7.

Similar as for the single defect we see that the cutoff is increased and the modulating structure in the enveloping function becomes more emphasized when we move towards the relativistic regime. In addition we note that the difference between the even and odd harmonic becomes larger with increasing U_p. This effect is more extreme for the low order harmonics. As a general observation we state that there are not any effects which seem to be special to the relativistic regime, but the transition to that regime seems to be rather smooth.

V. CONCLUSIONS

We have minimally coupled a laser field to an impurity system in a quantum wire described with the Dirac equation. Using a free field expansion for the free Dirac Fermion, we computed by means of standard potential scattering theory the reflection and transmission amplitudes associated to such type of defect. The amplitudes become functions of the defect coupling constant g, their separation y, and the laser field parameters E_0, ω, and t. We employed these amplitudes in order to evaluate the emission spectrum of a dipole moment in such a system. Our findings for a single defect, taken to be the energy operator coupled minimally to the laser field, are that even multiples of the driving frequency ω are emitted. Investigating a double defect system of two of such defects, we observe the emission of odd as well as even multiples of the original frequency. These features may already be observed qualitatively on the Fourier expansion of the transmission amplitude, even analytically. When carrying out the nonrelativistic and extreme relativistic limit we do not observe any special effect, the transition seems to be rather smooth.

There are various questions left for further investigation. As an interesting application one may for instance compute the conductance in a similar fashion as in Ref. 10 and employ the laser to control it.

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