High harmonic generation in time-dependent quantum box

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We consider optical harmonic generation in time-dependent box driven by external time-periodic field. Two types of the external field is considered: Time-periodic optical field and a field created by harmonically oscillating wall of the box. The latter is treated on in terms of the Schrodinger equation with time-dependent boundary conditions.

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I. INTRODUCTION

Quantum particle dynamics in time-dependent traps such as hard wall box, cavity and well attracted much attention during past few decades \cite{1,2}. Modern technological developments allow trapping and manipulating of particles in time-dependent potentials, including those which can create very high barriers making impossible particle escape. Manipulation of the particle dynamics is of practical importance in such field as metrology and quantum information processing. Possibility for creating of time-dependent traps and confining there particles and atomic bound states have been discussed recently in different contexts \cite{1,2}. In most of the cases confinement is created by optical potential that causes additional effects of particle-wall interaction, such as pressure, compressing of the confined particle, acceleration, optical harmonic generation, etc. In other words, interaction of confined particles with the moving boundary causes modification of the boundary conditions making them dynamical that leads to different dynamical effects which does not appear in case of the static confinement. The problem of moving boundaries in quantum mechanics is treated in terms of the Schrödinger equation with time-dependent boundary conditions. Earlier, the quantum dynamics of a particle confined in a time-dependent box was studied in different contexts (see Ref. \textsuperscript{6}-\textsuperscript{24}).

In this paper we consider optical harmonic generation caused by the interaction of confined particles with the harmonically oscillating wall by focusing in the role of confinement. We note that earlier, the optical harmonic generation in confined systems has been studied in different context (see, e.g., Refs. \textsuperscript{25}-\textsuperscript{30} and book \textsuperscript{31}). Pioneering treatment of the nonlinear effects, including harmonic generation dates back to the Ref. \textsuperscript{31}, where optical nonlinearity in asymmetric quantum wells due to resonant intersubband transitions are studied within the compact density-matrix approach. In \textsuperscript{27} similar problem is studied for nonparabolic two-level quantum well systems by taking into account depolarization effects. In \textsuperscript{28} a systematic procedure for the optimal design of quantum-well structures, which provide maximal resonant second-order susceptibility is proposed. Different nonlinear optical properties of in semiconductor quantum well are studied in \textsuperscript{31,32,33}. Optical rectification, second- and third-harmonic generations in a semispherical quantum dot placed at the center of a cubic quantum box are studied in \textsuperscript{38}. Despite the fact that different aspect of nonlinear optical phenomena in confined quantum systems are studied, most of the researches are restricted by considering the case of static confinement. However, dynamical confinement appears in many nanoscale systems and low-dimensional functional materials, where optical processes play important role. Here we study the role of dynamical confinement in high harmonic generation in confined quantum system by considering static and dynamic confinements. The latter is assumed to be created by moving wall of the box. This can be achieved, e.g., when confinement is caused by optical field, e.g., in atom optic billiards or tweezers. Since in most cases such oscillating trap can be created by optical field, interaction of the moving wall with the confined particles can cause nonlinear optical phenomena such as harmonic generation. The paper is organized as follows. In the next section we consider the problem of optical harmonic generation in 1D quantum box driven by external monochromatic field. In section III similar problem is considered in a quantum box with harmonically oscillating walls. Section IV presents some concluding remarks.
II. HARMONIC GENERATION IN DRIVEN QUANTUM BOX

Consider first the case of quantum particle confined in an impenetrable box of size $L$ and driven by external linearly polarized monochromatic field with the strength $F$ and frequency $\omega_0$. Such system can be described by time-dependent Schrödinger equation which is given by ($\hbar = m = e = 1$)

$$i \frac{\partial \Psi}{\partial t} = \left( -\frac{1}{2} \frac{d^2}{dx^2} - F x \cos \omega_0 t \right) \Psi, \quad 0 < x < L, \quad (1)$$

for which the (box) boundary conditions for $\Psi(x, t)$ are imposed as

$$\Psi(0, t) = \Psi(L, t) = 0. \quad (2)$$

Solutions of Eq. (1) can be expanded in terms of the complete set of the unperturbed box eigenfunctions as

$$\Psi(x, t) = \sum_n C_n(t) u_n(x), \quad (3)$$

where $u_n(x)$ are the eigenfunctions of the quantum particle confined in 1D box to be found from

$$H_0 u_n = E_n u_n. \quad (4)$$

Explicitly, $u_n$ and $E_n$ can be written as

$$u_n = \sqrt{\frac{2}{L}} \sin \frac{\pi n x}{L}, \quad (5)$$

and

$$E_n = \frac{\pi^2 n^2}{L^2}. \quad (6)$$

The functions $u_n$ fulfill the orthonormality condition given by

$$\int u_m^* u_n dx = \delta_{mn}, \quad (7)$$

For expansion coefficients, $C_n(t)$ using Eq. (1) we have system of first order differential equations given by

$$i \dot{C}_n(t) = E_n C_n - F \sum_n C_m(t) V_{mn} \cos \omega_0 t, \quad (8)$$

where

$$V_{mn} = \int x u_m^* u_n dx. \quad (9)$$

We are interested in the study of optical harmonic generation in the system described by Eq. (1). The main physical characteristics of such process is the average dipole moment which is given by

$$\bar{d}(t) = - \langle \Psi(x, t) | e x | \Psi(x, t) \rangle,$$

where $e$ is the electron charge.

Using Eqs. (3) and (7) one can write the average dipole moment as

$$\bar{d}(t) = - \sum_{m, n} C_m^* C_n(t) V_{mn},$$

where $V_{mn}$ is given by Eq. (9). The spectrum of harmonic generation is given by

$$\bar{d}(\omega) = \frac{1}{T} \int_0^T e^{-i\omega t} \bar{d}(t) dt, \quad (10)$$
where $T = 2\pi/\omega$.

In Fig. 1 $|d(\omega)|^2$ which determines the intensity of harmonic generation, is plotted at different values of the box size, $L$ for the values of external field amplitude and frequency, $F = 1$ and $\omega_0 = 0.1$ (a), $\omega_0 = 1$ (b). The intensity decreases, as the harmonic order increases for all values of $L$. Also, increasing of the frequency of external field does not change the situation, i.e., $|d(\omega)|^2$. In Fig. 2 $|d(\omega)|^2$ is plotted for the different values of external field strength, $F$ for $L = 15$ and $\omega_0 = 1$. The intensity decreases as the harmonic order increases. However, for higher field strengths the decrease is slower compared to lower values of $F$. All this implies that driven static quantum box is not interesting from the viewpoint of higher order harmonic and attosecond pulse generation. Therefore in section III we consider harmonic generation quantum box induced by dynamical confinement.

### III. TIME-DEPENDENT QUANTUM BOX

Consider quantum article confined in a 1D box with moving (right) wall, i.e., the position of the right wall is given by $L(t)$. Dynamics of such particle is governed by the time-dependent Schrödinger equation given by

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{1}{2} \frac{\partial^2 \psi}{\partial x^2}.$$  \hfill (11)

The boundary conditions for this equation are imposed as

$$\psi(x, t)|_{x=0} = \psi(x, t)|_{x=L(t)} = 0$$ \hfill (12)

To solve Eq. (11) one should transform the boundary conditions into time-independent (static) form. This can be done by new coordinate, $y$ which is given by

$$y = \frac{x}{L(t)},$$

and using the transformation of the wave function

$$\psi(y, t) = \sqrt{\frac{2}{L}} e^{\frac{i L y^2}{\hbar}} \varphi(y, t).$$ \hfill (13)

together with the time scaling given by

$$\tau = \int_0^t ds \frac{L(s)}{[L(s)]^2},$$

we can rewrite Eq. (11) as

$$i \frac{\partial \varphi}{\partial \tau} = -\frac{1}{2} \frac{\partial^2 \varphi}{\partial y^2} + \frac{1}{2} L^3 \ddot{L} y^2 \varphi.$$ \hfill (14)

Time and coordinate variables in Eq. (14) is possible only for the case, when $L(t)$ fulfills

$$L^3 \ddot{L} = \text{const.}.$$ 

For arbitrary time-dependence of $L(t)$ the problem can be solved only numerically, e.g., by expanding $\varphi(y, t)$ in terms of the complete set of eigenfunctions of a quantum box of unit size:

$$\varphi(y, t) = \sum_n C_n(t) \phi_n(y),$$ \hfill (15)

where $\phi_n(y)$ can be found from the following Schrödinger equation:

$$-\frac{1}{2} \frac{d^2 \phi_n}{dy^2} = E_n \phi_n,$$ \hfill (16)

with the boundary conditions

$$\phi_n|_{y=0} = \phi_n|_{y=1} = 0.$$ \hfill (17)

Explicitly, $\phi_n(y)$ can be written as

$$\phi_n(y) = \sin \pi n y$$ \hfill (18)

Then for the expansion coefficients we will have system of the first order differential equations:

$$i \sum \dot{C}_n \phi_n = \sum_n C_n E_n \phi_n + \frac{1}{2} L^3 \ddot{L} y^2 \sum_n C_n \phi_n.$$ \hfill (19)
including 4 different frequencies as

\[ \frac{1}{2} (A + B \cos \omega_0 t + C \cos 2 \omega_0 t + D \cos 3 \omega_0 t + E \cos 4 \omega_0 t) y^2 \]  

(21)

where

\[ A = -\frac{3b^2 \omega_0^2}{8} (4a^2 + b^2), \quad B = -\frac{3ab \omega_0^2}{4} (4a^2 + 9b^2), \]

\[ C = -\frac{b^2 \omega_0^2}{2} (3a^2 + b^2), \quad D = -\frac{3ab^3 \omega_0^2}{4}, \quad E = -\frac{b^4 \omega_0^2}{8} \]

Thus the virtual system can be considered as a quantum box with unit size and driven by nonlinearly polarized multichromatic field. The average dipole moment for such system can be written as

\[ \bar{d} = -\int_0^{L(t)} \psi^*(x,t) x \psi(x,t) dx = -2L \sum_{m,n} C_m^* C_n V_{mn}, \]  

(22)

where

\[ V_{mn} = \int_0^1 \phi_m^* y \phi_n^* dy \]  

(23)

In Fig.3 \(|d(\omega)|^2\) is plotted at different values of wall’s oscillation amplitude, \(b\) and for the values of initial position, oscillation frequency \(a = 10\) and \(\omega_0 = 1\), respectively. Decay of the intensity when the harmonic order increases can be seen from this plot, although for higher values of \(b\) the decay becomes slower.

Fig.4 presents plots of \(|d(\omega)|^2\) at different values of the wall’s oscillation frequency, \(\omega_0\) for the values of the wall’s initial position and oscillation amplitude \(a = 10\) and \(b = 5\), respectively. In general, the intensity decays rather slowly (compared to Figs. 1-3), when the harmonic order grows. However, the decay becomes very slow, for the higher values of \(\omega_0\). This result makes very attractive the dynamical traps, such as quantum box with harmonically oscillating wall, from the viewpoint of ultrashort pulse generation using optical high harmonic generation.

V. CONCLUSIONS

In this paper we considered the problem of optical high harmonic generation in confined quantum systems by considering the cases of static and dynamic confinements. The static system represents 1D quantum box driven by external linearly polarized monochromatic field. The intensity of harmonic generation is analyzed by computing numerically the average dipole moment as a function of harmonic order. The analysis of the case of static confinement shows that confinement does not lead to slowing done, or growth of the harmonic generation intensity. In
the case of dynamic confinement the wall of the box is considered as oscillating and created by an optical field, e.g. in atom optic billiards, or optical tweezers, where the oscillating wall plays the role of external field. It is found that when the wall’s oscillation frequency is large, the intensity of harmonic generation decays very slow as a function of harmonic order. The model studied in this paper can be useful for optical high harmonic and ultrashort pulse generation under dynamical optical confinement using, e.g., atom optic billiards.

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