Simulation of resonant high-order harmonic generation in a three-dimensional fullerenelike system by means of a multiconfigurational time-dependent Hartree-Fock approach

P. V. Redkin[1] and R. A. Ganeev[2]

[1]*Samarkand State University, 15, University Boulevard, Samarkand 140104, Uzbekistan,*

[2]*Institute of Electronics, Uzbekistan Academy of Sciences, Akademgorodok, 33, Dormon Yoli Street, Tashkent 100125, Uzbekistan*

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We performed a series of simulations of resonant high-order harmonic generation (HHG) by means of a multiconfigurational time-dependent Hartree-Fock (MCTDHF) approach for three-dimensional fullerenelike systems. The results proved the theory of resonant recombination proposed in this article and showed the ways of resonant HHG optimization. The results of MCTDHF calculation of the HHG for C_{60} were in good qualitative agreement with reported experimental data.

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I. INTRODUCTION

Resonant high-order harmonic generation (HHG) is the most efficient way to obtain coherent femtosecond pulses in the extreme ultraviolet and soft x-ray spectral ranges. The highest conversion ratio of pump energy into a single high harmonic is currently close to 10^{-4} [1]. In that regard, the fullerenes possessing strong surface plasmon resonances (SPRs) in the short wavelength range (~60 nm) now draw much attention as targets for resonant HHG. At the same time, note the absence of reports on higher-order harmonics in fullerenes until recent studies where the application of laser ablation allowed the production of plasma plumes containing considerable amounts of C_{60} particles for efficient conversion of the short laser pulses (i.e., of a few tens of femtoseconds) in the extreme ultraviolet (XUV) range [2–4]. In particular, for ablation of C_{60} film, estimates of the fullerene density in the ablation plume of no less than 5×10^{16} cm^{-3} were reported [2]. Broad SPRs of fullerenes also give the possibility of enhancing a group of neighboring harmonics, which is necessary for attosecond pulse train generation.

We have not found any report on successful resonant HHG in gases where a single harmonic dominates over the harmonic spectra. This can be explained by the much narrower range of available resonances in the XUV range for gases, as well as by the limited number of gases which can be used for HHG. In this regard, plasma ablation is an attractive way to create gaseouslike ionic media from most solid targets. This gives a greater possibility of finding a certain transition favorable for resonant HHG. Regarding this, we should say that plasma ablation gives a better probability of finding optimal transitions for resonant HHG compared to gases. At the same time note that no one can say for sure that plasma ablation should give the largest possible harmonic intensity. Plasma ablation of various targets is carried out by picosecond prepulses, which can be optimized by delay with regard to the main femtosecond pulse. A prepulse is not a disadvantage, as it requires only a beam splitter and helps us control the optimal conditions for HHG. In this approach, the application of prepulse allows the creation of monoparticle- and nanoparticle-containing plasmas, resonance-induced enhancement of harmonics, generation of extended plasma, etc.; that is, it gives the additional freedom of variation of nonlinear medium characteristics.

Theoretical studies of HHG from C_{60} involved extending the three-step model [5], analyzing an electron constrained over the surface of a rigid sphere, with geometrical parameters similar to those of the C_{60} fullerene [6], and using the dynamical simulations [7]. In the latter, higher-order harmonics were shown to be due to multiple excitations and could be easily generated even with a weak laser field. Both studies reveal how HHG can be used to probe the electronic and molecular structure of C_{60}. At the same time, theoretical investigation of such systems is hampered by the fact that the Hamiltonian of HHG is time dependent and the systems consist of many electrons. The investigation of influence of the fundamental properties of electrons on resonant HHG can be performed by means of a multiconfigurational time-dependent Hartree-Fock (MCTDHF) approach, which has the accuracy of direct numerical solution of Schrödinger equation and is almost as simple as the ordinary time-dependent Hartree-Fock (TDHF) approach. Our computations are based on the Heidelberg multiconfigurational time-dependent Hartree (MCTDH) software packages [8–10]. It can easily handle MCTDHF problems as well by setting all particles identical and the A vector of the wave function of the system fully antisymmetric in the initially unsymmetric MCTDH approximation.

In this article, simulations of resonant HHG are performed by means of a MCTDHF approach for three-dimensional fullerenelike systems. We analyze the influence of the SPR of C_{60} on harmonic efficiency in the range of 60 nm ($E = 20$ eV). These results showed the ways of resonant HHG optimization and, most important, attosecond pulse train generation. The MCTDHF calculations of the HHG for C_{60} were in good qualitative agreement with experimental data reported in previous studies of harmonic generation in fullerene-containing laser plumes.

II. THEORETICAL APPROACHES, RESULTS, AND DISCUSSION

The MCTDHF approach treats the wave function of a multielectronic system as

$$\Psi(Q_1,\ldots,Q_f,t) = \sum_{j_1=1}^{n_1}\cdots\sum_{j_f=1}^{n_f} A_{j_1}\cdots_{j_f}(t)\prod_{\kappa=1}^{f}\varphi_{j_\kappa}^{(\kappa)}(Q_\kappa,t), \quad (1)$$

where $Q_1,\ldots,Q_f$ are the coordinates of electrons and $A_{j_1}\ldots_{j_f}$ is the antisymmetrized A vector for all n_κ time-dependent expansion functions $\varphi_{j_\kappa}^{(\kappa)}$ for every degree of freedom κ. Setting $n_\kappa = n_1$ describes the direct solution of the time-dependent Schrödinger equation and $n_\kappa = 1$ simplifies the wave function to an ordinary TDHF approximation.

The equations of motion in the MCTDHF approach are derived from the modified variational principle:

$$\langle \delta\Psi_{\mathrm{MCHF}}(t)|\, i\frac{d}{dt} - H(t)\,|\Psi_{\mathrm{MCHF}}(t)\rangle = 0 \forall t. \tag{2}$$

The MCTDHF method was applied to simulate a three-dimensional fullerenelike system represented by the so-called jelliumlike sphere approximation. We used a jellium sphere as a potential surface for the representation of fullerenes. Then, two electrons were considered to be moving in this potential; that is, the remaining electrons were considered to be frozen. The system under investigation was represented by a spherically symmetric potential of the form [11] ($R_0 = 8.1$, $R_i = 5.3$, and $\upsilon_0 = 0.78$)

$$V(r) = \begin{cases} -3\left(\frac{250}{R_0^3 - R_i^3}\right)\left(\frac{R_0^2 - R_i^2}{2}\right), & r \leqslant R_i \\ -\left(\frac{250}{R_0^3 - R_i^3}\right)\left[\frac{3R_0^2}{2} - \left(\frac{r^2}{2} + \frac{R_i^3}{r}\right)\right] - \upsilon_0, & R_i < r < R_0, \\ -250/r, & r \geqslant R_0 \end{cases} \tag{3}$$

where $r = \sqrt{x^2 + y^2 + z^2}$ for both electrons.

The Coulomb repulsion between electrons was (2 is added to avoid singularity at 0)

$$V_{ee} = 1/\sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2 + 2}. \tag{4}$$

Later we present the results of the study of the interaction of the fullerenelike system with the Gaussian femtosecond electric pulse,

$$E(t) = \exp\left(\frac{(t - t_0)^2}{\tau^2}\right) E_0 \sin(\omega t), \tag{5}$$

where $\omega = 0.046$ atomic units (a.u., $\lambda = 991$ nm) or $\omega = 0.057$ a.u. ($\lambda = 800$ nm). The first frequency was chosen as a source of even (16^{th}) harmonic, which coincides with the central region of the SPR of C_{60} ($\lambda = 60$ nm), and the second frequency coincides with the frequency of the laser (Ti:sapphire) most frequently used in such experiments.

The simulation box size was 100 a.u. in each direction for each degree of freedom. The intergrid spacing was 0.1 a.u., which is quite sufficient (the particles are indistinguishable, so the main contribution comes from the A vector, if more than one configuration is considered). No further investigations of influence of mesh size on the results were performed, as we just needed to check the influence of configurations.

From the solution of MCTDHF equations for $\Psi(Q_1,\ldots,Q_f,t)$, the time-dependent dipole $d(t) = \sum_f \int \Psi(Q_1,\ldots,Q_f,t) Q_f \Psi^*(Q_1,\ldots,Q_f,t)$ was obtained for the estimation of the power spectrum of HHG. It is well known that, for analytically given expressions (such as in semiclassical approaches), the Fourier transform gives exact results as it treats all signals as quasi-infinite. But this turned out not to hold true for discrete Fourier transforms when analyzing extremely short signals due to the well-known fact of spectral leakage which is present for any possible window function, including a rectangular one.

That's why our piecewise least-squares approximation can be considered an efficient method for analysis of HHG on the basis of sampled time-dependent quantities. It consists of a least-squares approximation of $d(t)$ to a sum of harmonics on every sufficiently small time interval and summation of the resulting indices to get the resulting HHG spectrum $d(t) = \sum_{i=1}^{N} a_i \sin(b_i \omega t), N \leqslant T/dt$ (T is the pulse length, dt is the time step). Usually N is 2 or 3 times smaller than T/dt and b_i is $1+2i$. The analytical Fourier transform is simply the evaluation of an indefinite integral $S(\Omega) = \int d(t) e^{i\Omega t} dt$. However, discrete Fourier transform does not directly evaluate the corresponding definite integral $S(\Omega) = \int_0^T d(t) e^{i\Omega t} dt$. Instead, it tries to make the fit $d(t) = \sum_{i=1}^{T/dt} a_i \sin(a_i \omega t)$. Thus, discrete Fourier transforms, being another way of fitting the sampled data to sinusoids, can also be done piecewise, but the resulting set of fixed sampling frequencies will be determined only by the time step (which may be far from harmonics) and, most important, the fit is not guaranteed to be optimal and is not unique (although it's relatively exact then). At the same time, the fit obtained by means of least-squares approximation is always optimal by construction and unique. Its only disadvantage is that the frequencies of harmonics have to be guessed, although this is not too difficult if we know that the resulting spectrum should consist of harmonics only. Another advantage of this method is the fact that functions for approximation should not necessarily be pure sinusoids. Actually, our fitting functions were equally Gaussian-broadened sinusoids to take into account slight deviations from the monochromaticity of harmonics induced by the pump intensity modulation and by possible computational inaccuracies. The advantage of this method is not only its full mathematic correctness and accuracy but also the fact that the harmonic spectrum becomes easily viewable by definition.

The absorption spectrum of this system was obtained by a procedure similar to the δ-kick method [12]. It consists of applying to the whole system a strong rectangular pulse ($E = 0.01$ a.u.) in the beginning of propagation and then evaluating the free propagation of the system, after which the spectrum is obtained via Fourier transform of the $x_1(t)$. This approach is not implemented in the Heidelberg MCTDH package directly, so we simply used a user-defined field.

The spectrum had absorption maxima near 0.741 a.u. ($\sim$60 nm), which is approximately the 13^{th} harmonic of $\omega = 0.057$ a.u. radiation and the 16^{th} harmonic of $\omega = 0.046$ a.u. radiation, although the absorption band is rather wide (see inset in Fig. 1). We should mention that we consider a simple jelliumlike system, not the C_{60} molecule itself, so the spectrum may deviate from the experimental one.

Figure 1 presents the results of HHG simulation within exact MCTDHF approximation (six expansion functions) for carrier wave frequencies of 0.046 and 0.057 a.u. The 13^{th} harmonic of 0.057 a.u. radiation was approximately 10 times enhanced relative to the plateau harmonics. Note that the experimentally observed enhancement of this harmonic was approximately the same and depended on the excitation of fullerene-containing targets [2]. One can see that harmonics

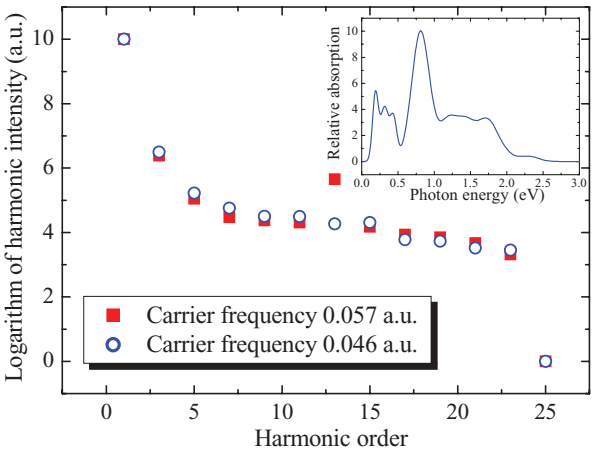

FIG. 1. (Color online) The influence of resonance on the HHG spectrum generating in fullerenelike medium in the cases of radiation of carrier wave frequencies 0.046 a.u. (open circles) and 0.057 a.u. (solid squares). Inset: Absorption spectrum of the fullerenelike system obtained by the δ-kick method.

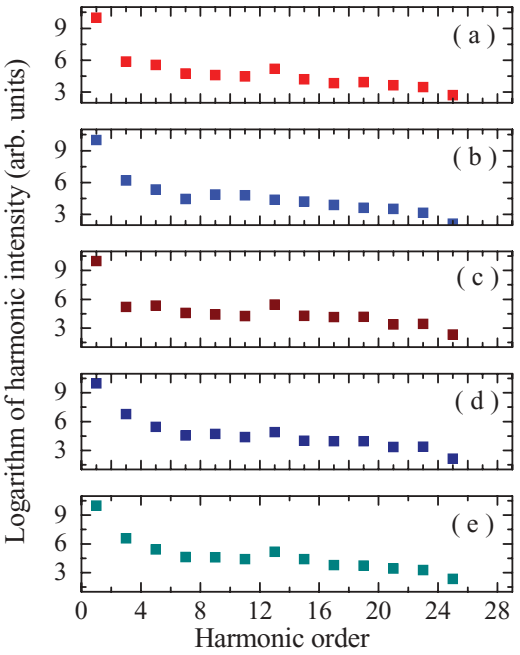

FIG. 2. (Color online) The influence of approximations on the observability of resonant HHG. (a) Without the influence of exchange, (b) without the influence of interaction, (c) six expansion functions, (d) three expansion functions, (e) one expansion function.

neighboring the 13th are not so enhanced, although they are still close to the broad absorption band of C_{60} (50–70 nm). At the same time, they are not suppressed, so it is highly possible that a competition between enhancement and absorption takes place. The pulse in general is not monochromatic, so its spectral properties can also have an influence on the simulations.

We also observed even harmonics, which were 2 orders of magnitude smaller than the neighboring odd harmonics. This artifact can be attributed to symmetry breaking introduced by the numerical grid, which is perhaps still too sparse and introduces some kind of rectangular integration box as well. Further reducing of the grid spacing may remove such an unphysical result. Note, that in contrast to the time-dependent density-functional theory (TDDFT) method, no spherically symmetric integration box can be introduced in the MCTDHF (at least, by means of the Heidelberg MCTDH package). However, these harmonics are almost 2 orders smaller than the odd ones and can be thus disregarded as some kind of numerical inaccuracy.

The resonant 13th harmonic of the radiation with carrier frequency $\omega = 0.057$ a.u. was enhanced. However, the 16th harmonic of the radiation with carrier frequency $\omega = 0.046$ a.u. was suppressed due to symmetry effects, which are still strong in our system. We should mention that in both cases the maximum observed harmonic order was 23, which is close to reported experimental results (19th and 25th harmonics [2–4]) at moderate excitation of fullerene-containing targets. All these results point out that the MCTDHF approximation indeed allows us to describe both resonant HHG and harmonic cutoff in the fullerenelike medium.

Then more simplified systems were studied under the same conditions for the Gaussian field with carrier wave frequency 0.057 a.u. The results of resonant HHG simulations in these approximations compared to results of MCTDHF calculations with six expansion functions are shown in Fig. 2. It is seen that reducing the number of configurations up to the TDHF approximation (i.e., one expansion function) did not lead to complete vanishing of resonant HHG, although the conversion efficiency of the resonant harmonic was reduced. In the one-dimensional case, when only a single coordinate of each particle was taken into account, the conversion efficiency of the resonant harmonic decreases as well. To sum it up, a large number of expansion functions is needed to observe resonant HHG in the one-dimensional case. However, the resonant nature of HHG for the 13th harmonic is unchanged by the number of configurations.

Two-electron interaction is a Coulomb repulsion [Eq. (4)] between two electrons. Neglecting the two-electron interaction resulted in nonresonant HHG without any significant suppression of other harmonics. At the same time the representation of quasielectrons as distinguishable particles had almost no influence on resonant HHG observability. The most important application of this phenomenon is the necessity of exact description of the two-electron interaction, while exchange processes have almost no effect on resonant HHG simulations. Probably some enhancement of the other harmonics observed in these calculations in the case of six exchange functions is determined by other resonant transitions in the system regarding dynamical modifications of the plasmon absorption spectrum.

These simulations, however, give no information about the origin of the resonant HHG process. According to the most widely accepted theory [13], resonant HHG is observed when there is a multiphoton resonance between the ground and excited states having different parities. Therefore there might have been a HHG process from the electrons, which left the excited state. The inevitable consequence of this theory is the enhancement of the harmonics neighboring the resonant one and this has not yet been proved by experiments. Here another theory is presented and it can in principle explain

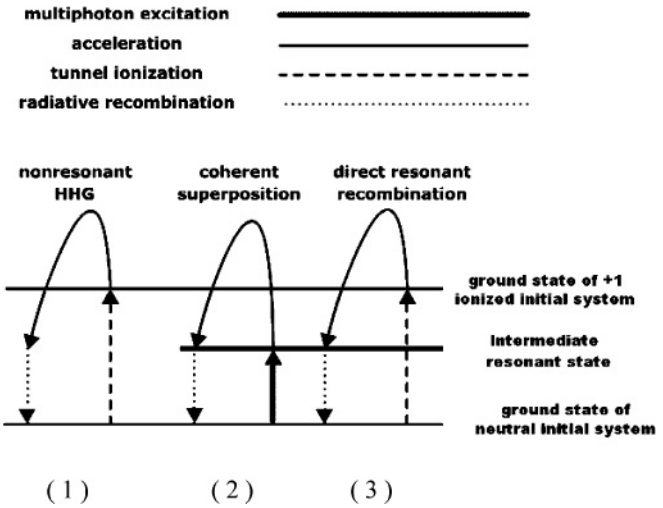

FIG. 3. Various scenarios of resonant and nonresonant HHG. (1) Nonresonant HHG case (ordinary three-step process); (2) HHG through the resonant multiphoton excitation [13]; (3) HHG from resonant recombination.

all the experimentally observed features of resonant HHG. This theory which we called direct resonant recombination theory consists of a strong increase in the single harmonic emission probability when the laser-induced energy level of the accelerated electron matches the resonant level of the system. The difference between the theory [13] and our direct resonant recombination theory is shown in Fig. 3, where a nonresonant case (1) is presented for comparison. One should note that, in Fig. 3, not the kinetic energy only, but the total energy is shown, so potential part of total energy obtained during tunnel or multiphoton ionization is also spent during recombination.

Let us compare our theory of direct resonant recombination [Fig. 3, case (3)] with the theory of harmonic generation from coherent superposition of states having different parities [13] [Fig. 3, case (2)]. As well as for nonresonant case [Fig. 3, case (1)], in our theory of direct resonant recombination [Fig. 3, case (3)], the electron is first ejected from the ground state by tunnel ionization (dashed arrow), whereas, in theory [13], the electron leaves the ground state due to resonant multiphoton excitation (solid arrow) to the excited state. Then, in all three cases, the electron accelerates in the field of laser radiation (solid curved arrows) and acquires the kinetic energy E_k. Further, the recombination of electron into the ground state with a HHG photon emission occurs.

The main difference between these theories is the following. In theory [13], resonances originate from the recombination into low-order even harmonics (0 or 2) with respect to the excited state, which stands in place of the ground state. Taking into account extremely high conversion efficiency for lower orders, such resonant enhancement is mainly determined by the efficiency of multiphoton transition. At the same time, direct resonant recombination gives us the emission of a single enhanced harmonic for any existing strong transition resonant with it and has almost no dependence on the excited state's population caused by multiphoton resonance.

The electron in the intermediate state is not supposed to be held too strongly, because the difference between this state and the ground state of the corresponding higher-lying ion is much smaller than in Fig. 3. However, this fact can be a counterargument to the theory of resonant HHG from coherent superposition of states [13], but by no means to our theory of direct resonant recombination.

Another fascinating peculiarity of our theory of resonant recombination is the fact that all the equations given in [13] can describe our theory as well without any changes. We can write the resulting expression for the induced dipole like in [13]:

$$\vec{d}_{jj'}(t) = -i\int_0^t dt' \int d^3\vec{q}\,\vec{d}_j^*(\vec{q}+\vec{A}(t))\vec{E}(t')\cdot\vec{d}_{j'}(\vec{q}+\vec{A}(t')) \times \exp[iS_{jj'}(\vec{q};t,t')] + \sum_{j,j'} a_j^* a_{j'}\langle j|r|j'\rangle \times \exp[-i(E_{j'}-E_j)t] \quad (6)$$

The only difference between theory [13] and our theory lies in the fact that the last term of Eq. (6), which is resonant, in our theory does not merely increase the effectiveness of ionization, as considered in [13], but plays the decisive role in the resonant recombination process, because its exact Fourier transform will give a contribution to the harmonic with frequency $E_{j'} - E_j$. So our theory can be easily explained semiclassically as well, giving us the full effectiveness of the semiclassical approach.

In order to check the correctness of these theories by means of numeric simulation, the time-dependent electric field was changed so that in the region of relatively low intensities (the beginning and the end of the pulse) the carrier wave had a frequency of 0.046 a.u., while in the region of higher intensities it had a frequency of 0.057 a.u. (see Fig. 4, open squares). For comparison the opposite case was considered in Fig. 4 (solid circles) where the carrier wave frequency was 0.057 a.u. for low intensities and 0.046 a.u. for higher intensities, respectively. No harmonic enhancement was observed in the former case. The results of HHG simulation showed that resonant HHG requires exact resonance at higher intensities first of all.

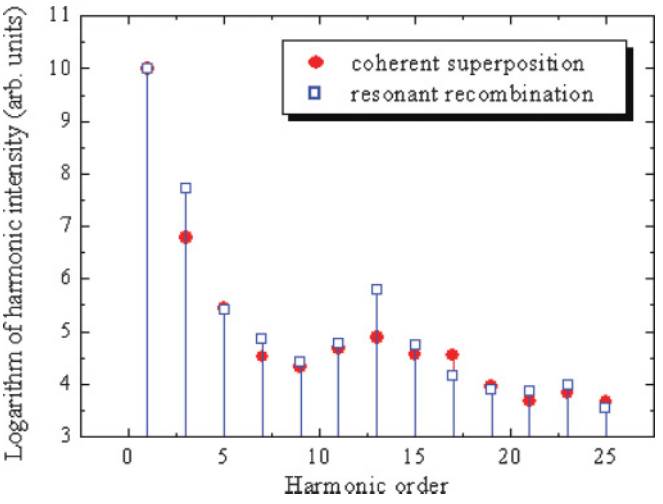

FIG. 4. (Color online) Results of simulation of the HHG for various deviations of carrier wave frequency from the resonant one for regimes favorable for coherent superposition or resonant recombination.

There are few recently published suitable theories that can explain resonant enhancement of a single harmonic. Some attempts in explanation of experimental observations have been reported in [13–16]. In particular, in [14], it has been shown that the influence of atomic autoionizing states on the phase matching of HHG may result in efficient selection of the single harmonic in calcium plasma. So, the real intensity enhancement can be even greater than that in single-atom approximation. An approach that suggests a HHG model describing enhancement of the generation efficiency for the harmonic resonant with the transition between the ground and the autoionizing state of the generating ion was developed in Ref. [15]. We should add that, although the autoionizing state is also a collective excitation, only the broadness of the SPR allows direct stimulated transition from the continuum into the ground state as in our theory, without additional need of radiationless transition, thus making possible competing enhancement of neighboring harmonics, which is useful for attosecond pulse train generation. In general, multielectron plasmon resonance of C_{60} is a generalization to two-electron autoionizing states in atoms and simple molecules; however, the extreme width of the plasmon resonance allows direct recombination, whereas for autoionizing states radiationless transition to these states should happen first. Usage of strongly ionized medium with some delocalized electrons as a target for resonant HHG can be favorable for extension of such attosecond pulse trains into the water-window region.

The results of numerical and analytical calculations based on this model are in quantitative agreement with those of the experiments showing HHG enhancement up to 2 orders of magnitude. In [16], it has been found that the laser intensity dependence of the intensity and phase of the single harmonic generated in resonant HHG from plasma ablation is different than that of the standard plateau and cutoff high harmonics. The resonant harmonic intensity increases continuously (i.e., without rapid oscillations) with the increase of the laser intensity, while the resonant harmonic phase is almost constant. Note that some recent experimental results contradict this conclusion.

Investigations of resonant HHG in multielectronic systems were also performed earlier for simplified systems by means of the MCTDHF approach by Zanghellini *et al.* (1D [17]) and Sukiasyan *et al.* (2D [18]). Despite the fact that both systems were greatly simplified and differ from our 3D case, both articles also revealed the importance of multielectronic effects. This can be used as an additional proof for our theory, where, despite that only one electron is actually accelerated in the laser field, the intermediate resonant state is required to be a collective multielectronic excitation such as the plasmon in this article or an autoionizing state for resonant HHG in indium vapors [19]. It is not evident how phenomena in C_{60} can be rescaled to the reduced dimensionality, although it might have interest of its own. Most TDDFT research also studies even the simplified jellium-sphere approximations for C_{60} in 3D [6], although reducing its dimensionality could result in speeding up computation time.

As a general conclusion, in any time-dependent HHG calculation which supports strong excited states, a resonant HHG should be observed if resonant conditions are met at the moment of recombination. The states themselves can be artificially introduced for single-electron models [15] or can follow naturally from potential well structure in multielectronic calculations. The scheme of direct resonant recombination presented in Fig. 3 for the corresponding initial system and $+1$ ionized initial system should explain all such phenomena. As a result, the method used to solve the approximated Schrödinger equation can have only a quantitative effect on the system. The article [6] completed within the TDDFT framework is clear evidence of this idea.

It should be mentioned that direct application of the MCTDHF method to large systems is still too demanding because of exponential growth of computational resources with the increase of the number of particles. According to qualitative independence of resonant HHG observation from the method of solution of the approximated Schrödinger equation for a given system, the approaches, such as TDDFT, which scale almost linearly with the number of particles are quite valid to be chosen for further investigation of complicated multielectronic systems.

The disadvantage of a MCTDHF approach for investigation of HHG is an artificial symmetry breaking due to integration grids. This can lead to observance of even harmonics, but we did not take these even harmonics into consideration within our approach of piecewise least-squares approximation. The TDDFT approach, in turn, being a one-electron method, suffers from inaccuracy of correlation effects within all available functionals [20]. Introduction of nonlocal exchange-correlation functionals [21] can become a convenient softening of this drawback.

III. CONCLUSIONS

In conclusion, the results of MCTDHF simulation of the resonant HHG in three-dimensional fullerenelike system revealed the decisive factors for resonant HHG, proved the proposed theory of resonant recombination for systems with plasmon resonances and showed promising ways of the resonant HHG optimization for the needs of attosecond pulse train generation. These computations were found in good qualitative agreement with the experimental results reported so far. It was found that any method of numerical simulation of HHG will show resonant HHG picture if the resonant conditions are met in the moment of recombination and the method supports corresponding strong resonant states. We have discussed the peculiarities of this approach and compared them with existing theories of resonance enhancement of harmonics.

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