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Simulation of Ultrafast Optical Transitions using Genetic Algorithm

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Abstract

The purpose of this paper is to investigate the possibility of application of the genetic algorithm to quantum control of electronic transitions between energy bands in solids. In particular, the hole transitions between valence bands induced by ultrashort (femtosecond duration) electric field pulse will be considered. Examples are presented to illustrate the efficiency of the algorithm in this case.

Keywords: electronic transition, energy bands, genetic algorithm.

1 Introduction

The problems of controlling various physical processes often are treated within a framework of traditional optimization theories. However their scope is limited, if control problems are complex or cannot be formulated in classical mechanics terms. One of relatively new statistical algorithms in practical optimization is the genetic algorithm (GA), which has originated from the studies of cellular automata conducted by J. Holland [1] and developed later by E. Goldberg [2]. More recent bibliography on GA can be found in books [3, 4] or on the server site [5].

If the response surface of the system is fairly simple, as mentioned, conventional nonlinear optimization and control theory techniques are acceptable. However, for many practical problems the response surface is difficult to search, for example, due to high-dimensionality, discontinuities, noisy input functions, quantum mechanical nature of the problem. In this case metaheuristic methods such as simulated annealing, GA, or messy GA algorithms are more suitable [3, 4].

In the last decade the GA was applied to rather diverse optimization problems such as laser control of chemical reactions [6, 7, 8], design of multilayered absorbing coatings for military planes that are invisible to radars [9], simulation of electron transport in semiconductors at high electric fields [10], retrieval of optical parameters in optical measurements [11], cutting stock problems, where minimization of scrap in cutting various widths of paper from large rolls is desirable [12].

Recently it was demonstrated that with the help of GA one can optimize shape of an ultrashort light pulse propagating in a single-mode optical fiber so that dispersion is not detrimental for such optical pulse propagation. GA generated optical pulses have rather complicated shape but they could be transmitted over much larger distances without loss of intensity and pulse width as compared to conventional optical pulses [13].

Here we are interested in application of the GA in obtaining femtosecond pulses that optimally control the electronic quantum transitions between energy bands in semiconductors. The target of the GA algorithm is to find such a shape of ultrashort radiation pulse which transfers the quantum particle from lower to upper energy band with as large as possible probability and at the same time the pulse energy remains as small as possible. In Sec. 2 the problem is formulated in terms of genetic algorithm and in Sec. 3 some representative simulation examples, where the algorithm is used to optimize the parameters of the electric field pulse, are presented.

2 Formulation

The following time-dependent Schrödinger equation written in atomic units was solved

$$i\frac{\partial|\psi\rangle}{\partial t} = (H_0 + \frac{\mathbf{F}(t)}{i}\frac{\partial}{\partial \mathbf{k}})|\psi\rangle, \tag{1}$$

where $i = \sqrt{-1}$. The equation (1) describes evolution of three-component vector $|\psi\rangle$ in the Hilbert space under control of arbitrary time-dependent electric field $\mathbf{F}(t)$ in three dimensional vector space. In (1), H_0 is the valence band Hamiltonian which in zero spin-orbit interaction limit is [14].

$$H_0 = \frac{1}{2}\begin{vmatrix} Nk_x^2 + M\mathbf{k}^2 & Nk_xk_y & Nk_xk_z \\ Nk_xk_y & Nk_y^2 + M\mathbf{k}^2 & Nk_yk_z \\ Nk_xk_z & Nk_yk_z & Nk_z^2 + M\mathbf{k}^2 \end{vmatrix} \tag{2}$$

where k_i is the projection of the hole wave vector $\mathbf{k}$ on the Cartesian axes, $i = x, y, z$, and N, M are the valence band parameters. The values M=12 and N=2 were used in the present simulation. Although the Schrödinger equation is linear with respect to wave function, it is nonlinear with respect to pertubation term, i.e., time-dependent electric field. The Hamiltonian (1) yields the following nondegenerate light (l) and doubly degenerate heavy (h) mass eigenenergies (dispersion laws)

$$\varepsilon_l = (M + N)\mathbf{k}^2, \tag{3}$$

$$\varepsilon_h = M\mathbf{k}^2. \tag{4}$$

The considered Hamiltonian has spherical symmetry, therefore, for simplicity the electric field was assumed to have only x component. Then, only k_x component will change with time and will obey the equation

$$dk_x/dt = F_x(t), \tag{5}$$

which in fact is one of the characteristic equations of (1). Using the characteristic equations the partial derivatives in (1) can be transformed to total derivative. As a result, the equation (1) may be reduced to

$$i\frac{d|\psi\rangle}{dt} = H_0(\mathbf{k})|\psi\rangle, \tag{6}$$

where time-dependence of $\mathbf{k}$ is described by (5). The components k_y and k_z do not vary with time in our case. The probabilities to detect the hole in light $p_l(t)$ and heavy $p_h(t)$ mass bands at the moment t can be calculated from the state vector $|\psi(t)\rangle$ using appropriate time-dependent unitary transformation matrix $T(t)$

$$|f(t)\rangle = T(t)|\psi(t)\rangle, \langle f(t)|f(t)\rangle \equiv |f(t)|^2 = \sum_{j=l,h1,h2} |f_j(t)|^2 = 1. \tag{7}$$

The last equality in (7) expresses the normalization condition of the state vector in the Hilbert space. Then the probabilities (or respective band populations) can be calculated from

$$p_l = |f_l|^2, p_h = |f_{h1}|^2 + |f_{h2}|^2. \tag{8}$$

The singular-value decomposition matrix which diagonalizes the Hamiltonian (2) was used to find unitary matrix $T(t)$ at equally spaced moments as described in [15].

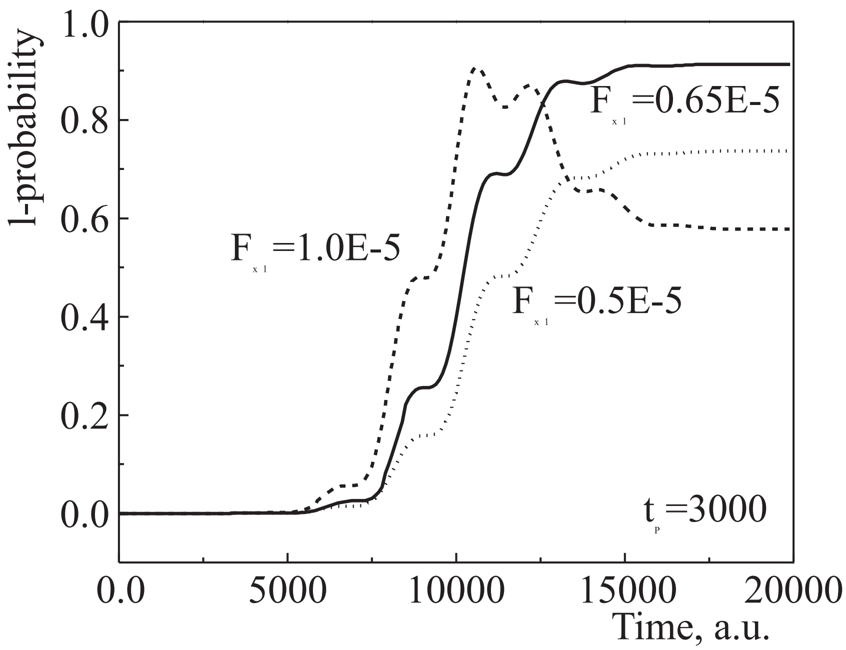

Fig. 1. Time dependence of the probability p_l to find the hole in l- band under Gaussian pulse excitation, equation (9), at various amplitudes: F_{x1}=0.5×10^{-5}, 0.65×10^{-5}, 1×10^{-5}. The other parameters are t_p =3000, t_d=10 000, ω=0.00135, α=0, φ=0.

Fig. 1 shows typical numerical solutions of the Schrödinger equation (1), when harmonically varying electric field pulse modulated by Gaussian envelope serves as a perturbation:

$$F_x(t) = F_{x1} \exp[-\log 2(\frac{t - t_d}{t_p})^2] \sin[\omega t + \alpha(t - t_d)^2 + \varphi]. \tag{9}$$

Here, F_{x1} is the amplitude, t_p is the halfwidth of the pulse, t_d is the delay, ω is the cyclic frequency, and φ is the phase. The coefficient α

takes into account chirping of the frequency. The Schrödinger equation was solved as an initial value problem, assuming at the moment $t = 0$ that the hole was in heavy hole mass band ($p_h = 1$, $p_l = 0$) and possessed the wave vector $\mathbf{k}_0$=(k_{x0}, k_{y0}, k_{z0})=$0.015(\sqrt{0.01},\sqrt{0.495},\sqrt{0.495})$. To enhance the transition probability the frequency ω was equated to transition energy at wave vector $\mathbf{k}_0$: $\omega = \varepsilon_l(\mathbf{k}_0) - \varepsilon_h(\mathbf{k}_0)$=0.00135. In the Fig. 1 one can see that there is an optimum electric field amplitude for the probability $p_l(t_f)$ at the final moment t_f=20 000 to reach the maximum value.

It should be noted that in general case the probability $p_l(t_f)$ depends on the overall shape of the electric field and can have many minima and maxima on the response surface. A related problem of finding an optimal shape of the electric field was recently solved using the direct optimization method of nonlinear programming [16].

In general, the problem of quantum control may be multivalued, since according to considerations of [17] there may be "denumerably infinite number of solutions to well-posed quantum-mechanical optimal-control problems". In the present work we have solved a simpler control problem, in which the form of the electric field is assumed beforehand and only a finite number of parameters is varied to achieve the best cost function, or fitness in terms of genetic algorithm defined as

$$\Phi = \max[|f_l(t_f)|^2 - a\int_0^{t_f} F^2(t)dt] \tag{10}$$

in the present work. The second, integral term in (10) is the penalty function. The coefficient a is an arbitrary constant, that limits the total energy of the radiation field. Thus, to satisfy the condition (10) one must find such a form of the electric field pulse which simultaneously satisfies two conflicting requirements: the energy of the pulse should be minimal but the transition probability at the end of the pulse should be maximal.

Fig. 2 illustrates schematically the GA algorithm for finding the best set of parameters in (9) that maximize the fitness function (10). In genetic algorithm one considers a population of possible solutions that consists of chromosomes or individuals (various sets of parameters $F_{x1}, t_p, \omega, \alpha, \varphi$, in our case).

The best set is found by selection, crossover and mutation operators applied to successive generations of the population. The chromosomes within a single population are encoded as strings of bits called genes. In our case a single string consists of $15n_p$ bits, where n_p is the total number of varied parameters. The number 15 means that in the present problem every parameter can assume 2^{15} different values. In our algorithm the gene is allowed to assume either 0 or 1 value. The latters are called alleles.

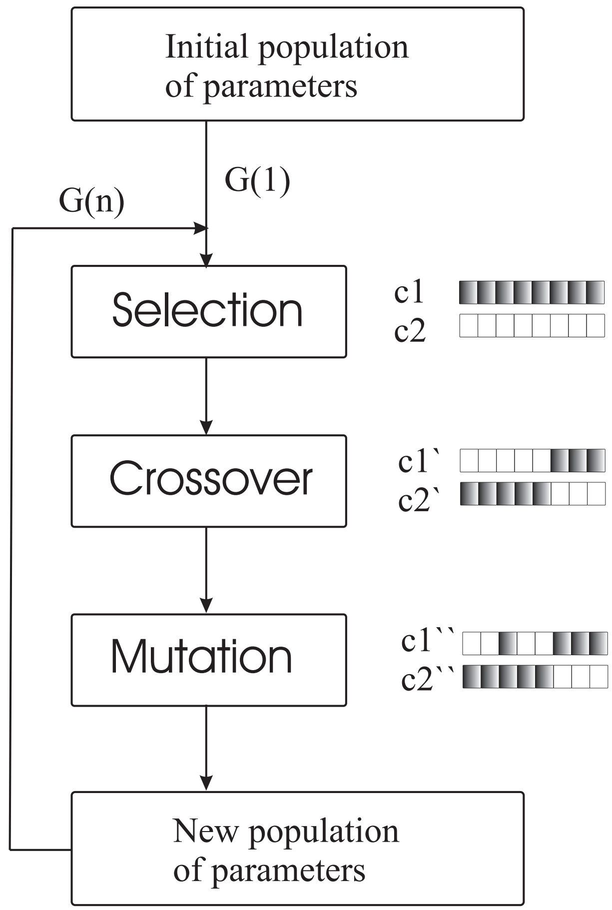

Fig. 2. Schematic of production of a new generation in the present genetic algorithm. On the right-hand side the selection, crossover and mutation operators over two chromosomes (individuals) of the population are shown as 0 and 1 bits.

In the first generation the genes were filled with random zeros and ones and later were changed during implementation of the GA. In the simulation we have used five individuals in population. Every new generation was renovated after operations shown schematically in Fig. 2 were performed over entire population. The selection operator sorts the population in order of fitness defined by (10). After evaluation of the fitness of each chromosome, a new population (offspring) is formed from the old one via the following two-step process.

In the crossover the fittest individuals interchange their genes according to the genetic material of the parents. Uniform crossover with the crossover probability equal 0.5 was used in the present algorithm. This means that two chromosomes are cut into two parts with the probability 0.5 at random position of the chromosomes, and then the partners exchange their sections as shown schematically on the right-hand side of Fig. 2.

The other important GA operator is mutation, during which the value of a bit at a randomly chosen position of the string is changed from 0 to 1 or from 1 to 0. A jump mutation was used with the mutation probability 0.02. The mutation operation, speaking popularly, brings fresh blood in the subsequent generations, or in mathematical terms the mutation does not allow the solution to be trapped in a local extremum. Elitism was incorporated in the present GA, so that the best individuals were not lost and replicated into the next generation. Now that we have described the GA, in the next section the efficiency of the algorithm will be illustrated in the interband-transition quantum-control problem.

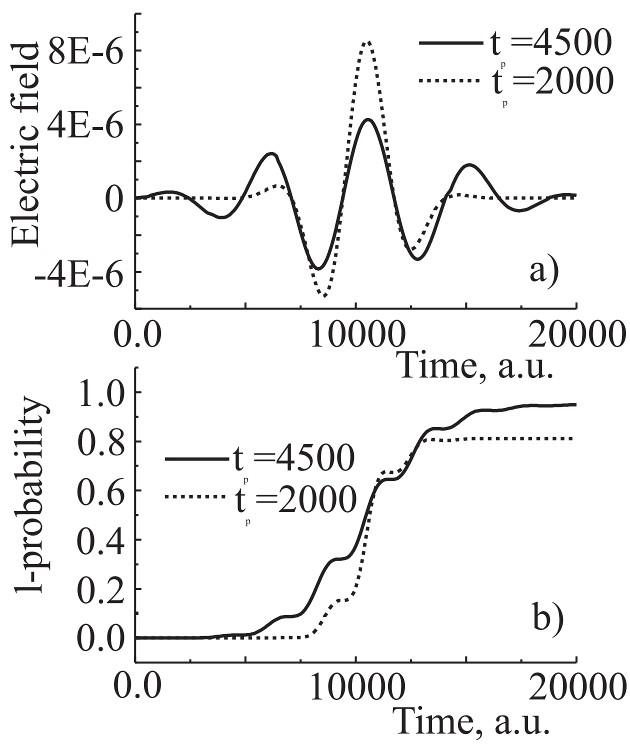

Fig. 3. Optimal electric field and the probability to find the hole in the light mass band as a function of time at two pulse halfwidths, t_p=2000 and 4500. Only F_{x1} was varied in the genetic algorithm in this case.

3 Examples

The Fortran program that was used to solve the above discussed problem consisted of two parts, of GA solver and of Schrödinger equation solver. The solvers were called one after another. The loop was terminated after a prescribed number of iterations has been performed. First, simple case where optimal solution depends on a single parameter only will be considered.

Fig. 3 shows the optimized shape of electric field and time-dependence of the probability $p_l = |f_l(t)|^2$ for a hole to be in the light mass band at two pulse halfwidths, t_p=2000 and 4500. Only F_{x1} was optimized to satisfy the condition for the best fitness. The other parameter values were constant as in Fig.1. From Fig. 3 it is seen that a wider pulse having smaller amplitude gives larger final probability $p_l(t_f)$.

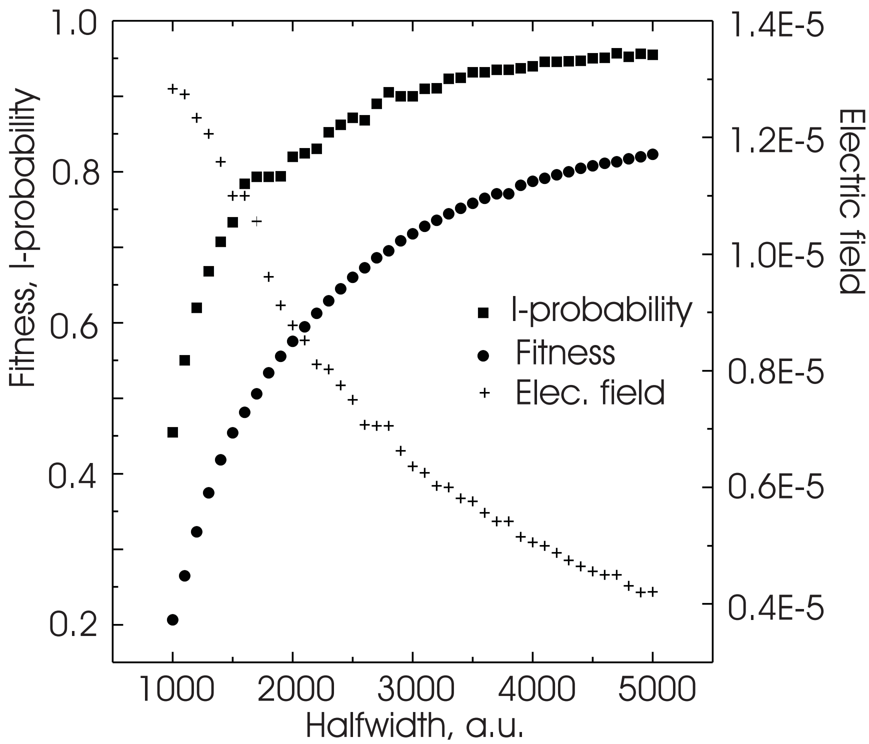

Fig. 4. The best fitness Φ, probability at final time $p_l(t_f)$ and electric field amplitude F_{x1} versus pulse halfwidth. Only F_{x1} was varied in the genetic algorithm in this case. a=0.2×10^7.

Fig. 4 shows the dependence of $p_l(t_f)$, best fitness Φ and amplitude F_{x1} on the pulse halfwidth. Wider electric pulses, in accordance with general considerations, require smaller F_{x1} values to transfer the hole to light mass band.

However, in case of extremely short pulses when $t_p \leq 2000$ (=48 fs) the final probability and the fitness decrease drastically as the pulse with is shortened. Such behavior indicates that the shape of the controlling electric field is far from optimal.

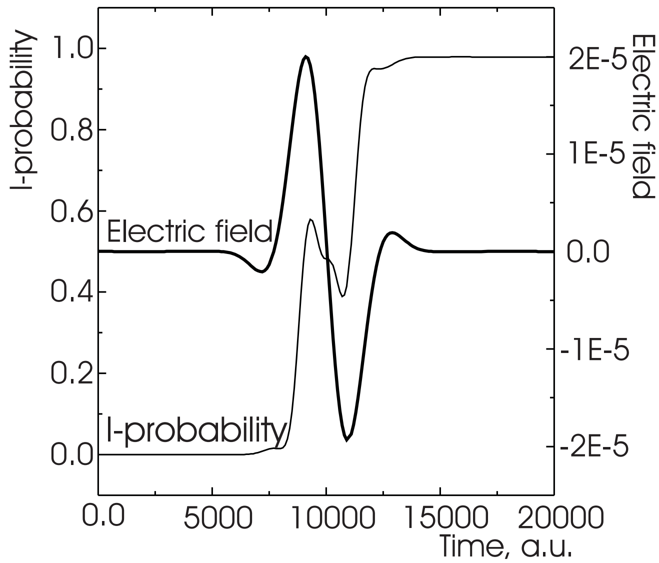

Fig. 5. The shape of the optimal electric field and the probability p_l versus time when four parameters F_{x1}, t_p, α, and φ are varied.

Fig. 5 shows the pulse shape and the probability when four parameters were allowed to be varied in GA in the range: F_{x1}=(1.2-3.6)$\times10^{-5}$, t_p=(1-2)$\times10^{3}$, φ=(0-π) and α=(0.05-0.3)$\times10^{-8}$. The central frequency remained fixed to resonance value, ω=1.35$\times10^{-3}$. The genetic algorithm yielded the following optimal values: F_{x1}=2.6$\times10^{-5}$, t_p=1625, φ=2.16 and α=0.187$\times10^{-8}$. After 80 generations the final probability was $p_l(t_f)$=0.978 and the best fitness was Φ=0.819 at a=0.2$\times10^{6}$. Fig. 6 shows the dependence of the best fitness Φ and averaged over single population fitness Φ_{av} as a function of generation number.

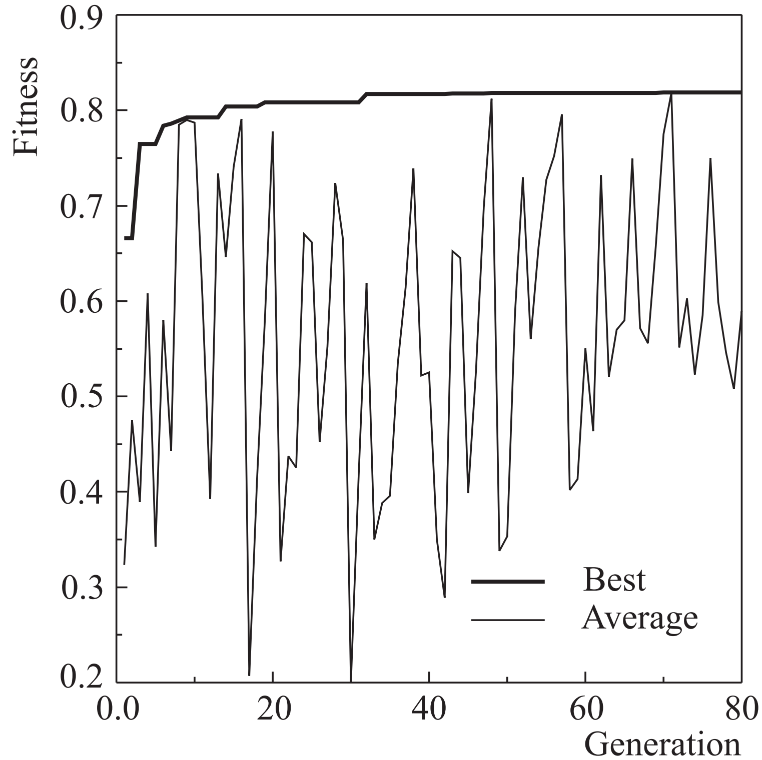

Fig. 6. The best and average fitness as a function of generation number.

The best fitness rises steeply with the generation number and then slowly saturates as the global maximum is approached. This is a normal behaviour found in most genetic algorithms [3]. However, the average Φ_{av} has a chaotic character. This is due to mutation operator. The mutation probes various regions, which sometimes may be at large distances from the global maximum, in the four-dimensional parameter space.

The mutation operation is required by the algorithm, in order for it to know whether the maximum is indeed global and that the subsequent probing points have not stuck in one of local extrema. The considered GA, in addition to electric pulse optimization in the Schrödinger equation, also allows to search for optimal coefficients in the fitness function (10). For example, in the considered case one can try to include the coefficient a in the bits of the chromosome, and thus rather easily transform the program to the dynamical optimization program, where optimization conditions are controlled during implementation of the genetic algorithm. Of course, in the considered example this has no sense, since the genetic algorithm with respect to a is not stable: the program tries to eliminate the second term in (10) by pushing a value to zero.

In summary, it was shown that genetic algorithm can be used in finding optimal ultrashort pulses which induce coherent transitions between energy bands in semiconductors. A satisfactory solution can be reached after probing 20-40 points in the multiparameter space and after integration of the Schrödinger equation at these points. This negligible number of points is to be compared to the total possible number of solutions, which is equal $(2^{15})^4 \approx 1.15\times10^{18}$ in the considered four-parameter space. The genetic algorithm was found to be very robust and relatively fast for not too large number of the probing points. In [16] the same quantum problem was solved in a different way, using the constrained minimization algorithm.

The latter algorithm relies on analytical methods (rather than on statistical methods as GA does) to find the global maximum. Due to restricted class of the functions generated in the present GA, it was impossible to compare directly the present results with those obtained earlier using the constrained minimization algorithm, where much wider class of control functions was generated. The considered genetic algorithm should be generalized in this case to include larger class of possible functions. In conclusion, the present work shows that the genetic algorithm can be used to generate the shapes of electric fields which induce ultrafast intervalence charge carrier transitions.

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