Quantum-well shape optimization for intersubband-related electro-optic modulation properties

J. Radovanović, V. Milanović,* Z. Ikonić, and D. Indjin
Faculty of Electrical Engineering, University of Belgrade, Bulevar Revolucije 73, 11120 Belgrade, Yugoslavia
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A method is described for the optimized design of quantum-well structures, in respect to maximizing the second-order susceptibilities relevant for electro-optic applications. It relies on applying the isospectral (energy structure preserving) transformations to an initial Hamiltonian, in order to generate parameter(s) controlled family of Hamiltonians that (i) are isospectral to the initial one and, (ii) have the potential variation proportional to the effective mass variation, being thus realizable by graded ternary alloys like $Al_xGa_{1-x}As$. By changing the values of control parameters one changes the potential shape and thus the values of matrix elements relevant for the susceptibility to be maximized. The use of the method is demonstrated by designing optimal quantum wells for the Stark effect or quantum interference derived electro-optical effects.
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I. INTRODUCTION

There has been a very intense research activity in the past decade in the field of intersubband-transitions-based optical effects in semiconductor quantum wells.[1–4] The dipole matrix elements that characterize such transitions are of the order of the quantum well (QW) width, i.e., a few nm, well above those in atoms or molecules. Large matrix elements generally lead to significant optical nonlinearities, particularly if these are enhanced by meeting the resonance conditions. In view of remarkable ''tailorability'' of QW electronic structure and related properties, the design of QW's highly matched to a particular application should be possible. Among the most interesting perspective applications of QW structures is the one for electro-optic modulators. It relies on the fact that both the absorption and the refractive index of QW's may be controlled by quasistatic electric field (so this formally is a nonlinear optical effect, described by second-order susceptibility). Modulation of absorption or the refractive index results in either amplitude or phase modulation of light, and is most efficient if the light is about resonant with some transition in the QW structure.

The applied electric field influences the QW in two ways, which both contribute to changing its index of refraction: it shifts the quantized electronic states (Stark effect), and it changes the values of various dipole matrix elements, by changing the wave functions of electronic states (this may be interpreted as field-induced mixing of wave functions and is often called quantum interference). For purpose of phase modulation, it seems that the quantum interference effect is advantageous over the the Stark effect.[4] In any case, for a specified wavelength of light and type of modulation, the QW shape may be designed to provide the most efficient modulation, i.e., the largest value of the corresponding second-order susceptibility.

In this paper we present a method for such optimized design of QW shape, which will maximize the electo-optic effect, in particular in ternary alloy based QW's (e.g., $Al_xGa_{1-x}As$). The method relies on some theoretical tools of quantum mechanics, which will first be described in Sec. II, and its use will be illustrated in Sec. III.

II. THEORETICAL CONSIDERATIONS

A. Intraband electro-optic susceptibility

Consider a QW of arbitrary shape, biased by an external dc field. Intraband transitions related electro-optic susceptibility may be determined by considering such a system as a new structure that interacts with the optical field in a linear manner, while the influence of the dc field is described implicitly, via bound states energies and wave functions, or density of states, that all depend on the bias field. The linear susceptibility of biased QW may then be written as[3]

$$\chi^{(1)}(\omega,K)=\sum_{i,j}\chi^{(1)}_{i,j}(\omega,K)=\frac{e^2}{\epsilon_0\hbar}\sum_{i,j}\frac{M_{ij}(K)M_{ji}(K)}{[\omega-\omega_{ij}(K)-i\Gamma_{ij}]}[N_j(K)-N_i(K)], \tag{1}$$

where $M_{ij}=\langle\psi_i|z|\psi_j\rangle$ is the dipole transition matrix element between states i and j, Γ_{ij} the off-diagonal relaxation rate, $\omega_{ij}=(E_i-E_j)/\hbar$, while $E_i,\psi_i=\psi_i(z)$, and N_i, respectively, denote the energy, envelope wave function, and electron density in the state i, while K is the quasistatic electric bias field. The summation is to be performed over all bound states of this QW. Equation (1) may then be expanded in Taylor series in K, and it suffices to take the constant and linear-in-K terms for further consideration, i.e.,

$$\chi^{(1)}(\omega,K)=\chi^{(1)}(\omega,0)+[\chi^{(2)}_S(\omega)+\chi^{(2)}_{QI}(\omega)+\chi^{(2)}_{CD}(\omega)]\cdot K+\cdots. \tag{2}$$

The three terms in brackets are the electro-optical coefficients of the structure, and are defined as

$$\chi_S^{(2)}(\omega)=\sum_{i,j}\left(\frac{\partial\chi_{ij}}{\partial\omega_{ij}}\frac{\partial\omega_{ij}}{\partial K}\right)_{K=0},$$

$$\chi_{QI}^{(2)}(\omega)=\sum_{i,j}\left(\frac{\partial\chi_{ij}}{\partial M_{ij}}\frac{\partial M_{ij}}{\partial K}+\frac{\partial\chi_{ij}}{\partial M_{ji}}\frac{\partial M_{ji}}{\partial K}\right)_{K=0},$$

$$\chi_{CD}^{(2)}(\omega)=\sum_{i,j}\left(\frac{\partial\chi_{ij}}{\partial N_j}\frac{\partial N_j}{\partial K}+\frac{\partial\chi_{ij}}{\partial N_i}\frac{\partial N_i}{\partial K}\right)_{K=0}. \tag{3}$$

The $\chi_S^{(2)}$ term originates from the linear Stark shift of QW states, while $\chi_{QI}^{(2)}$ appears as a consequence of changing the dipole matrix elements, due to the interference of envelope wave functions of bound states. Finally, $\chi_{CD}^{(2)}$ describes the bias-dependent redistribution of electrons over the QW states. With the field-electron interaction Hamiltonian written as $H_{int}=-eKz$, the first-order perturbation theory may be used to find the corrections to state energies and wave functions, which allow the Stark and quantum interference (QI) susceptibilities to be written as[3]

$$\chi_S^{(2)}(\omega)=\frac{N_1e^3}{\epsilon_0\hbar^2}\sum_{j\neq1}\frac{(M_1j)^2(M_{jj}-M_{11})}{(\omega-\omega_{j1}-i\Gamma_{j1})^2},$$

$$\chi_{QI}^{(2)}(\omega)=\frac{2N_1e^3}{\epsilon_0\hbar^2}\left[\frac{M_{12}M_{23}M_{31}}{\Delta_{21}(\omega-\omega_{21}-i\Gamma_{21})}+\frac{M_{12}M_{23}M_{31}}{\Delta_{31}(\omega-\omega_{31}-i\Gamma_{31})}+\frac{(M_{12})^2(M_{22}-M_{11})}{\omega_{21}(\omega-\omega_{21}-i\Gamma_{21})}+\frac{(M_{13})^2(M_{33}-M_{11})}{\omega_{31}(\omega-\omega_{31}-i\Gamma_{31})}\right]. \tag{4}$$

In these expressions the notation N_i, ω_{ij}, and E_i refers to unbiased QW, and it is also assumed that the majority of carriers resides in the lowest state, i.e., $N_1\gg N_j(j\neq1)$. Furthermore, the quantities Δ_{21} and Δ_{31} are defined as

$$\frac{1}{\Delta_{21}}=\frac{1}{\omega_{31}}+\frac{1}{\omega_{32}},\quad \frac{1}{\Delta_{31}}=\frac{1}{\omega_{21}}-\frac{1}{\omega_{32}}$$

.

In the QI-derived part of susceptibility, two distinct contributions may be noticed. One of these originates from the coherent interference of envelope functions of states directly involved in the optical transition, which constitutes type-I quantum interference, and is described by the third and fourth term in $\chi_{QI}^{(2)}$. The combination of matrix elements is here the same as in Stark-derived susceptibility. The first two terms in $\chi_{QI}^{(2)}$ describe the type-II quantum interference, comprising both the states that are directly involved in optical transition and those which are not (but still are necessary for this type of QI). QW's may be designed so that one of the above three parts of susceptibility dominates over the other two. Generally, one may write[3]

$$\frac{\chi_{QI}^{(2)}}{\chi_S^{(2)}}(\omega\approx\omega_{21})=2\left[\frac{\omega-\omega_{21}-i\Gamma_{21}}{\omega_{21}}+\frac{M_{23}M_{31}}{M_{21}(M_{22}-M_{11})}\frac{\omega-\omega_{21}-i\Gamma_{21}}{\Delta_{21}}\right]. \tag{5}$$

The first term in Eq. (5), representing the ratio of Stark and type-I QI susceptibilities is small at, or close to resonance, because $\Gamma_{21}\ll\omega_{21}$. Therefore, absent the interference with a third state , i.e., provided $M_{13}=0$ and $M_{22}-M_{11}\neq0$, the Stark effect would be dominant. One the other hand, if $M_{22}=M_{11}$ and $M_{13}\neq0$ the Stark effect would be negligible and type-II QI would dominate.

B. Isospectral transformations of the potential

It is clear from the above discussion that a QW has to be asymmetric if it is expected to have significant electro-optical coefficients. In symmetric structures one would have $M_{13}=0$ and $M_{11}=M_{22}$, due to definite parity of the wave functions, hence neither the Stark nor the type-II QI mechanisms would be effective. To maximize the electro-optical performance of a QW structure, its profile (i.e., the potential shape) should be varied in search for the largest $\chi^{(2)}$, of whatever type chosen. This optimization of QW profile can be classified as constrained, primarily due to the requirement that the QW states should be resonant with the incoming light. A convenient way of performing such optimization is via the supersymmetric quantum mechanics (SUSYQM).[5] This method enables one to start with an arbitrary 1D potential $U_1(z)$ and generate from it a family of potentials $U(\ldots,\lambda_j,\ldots;z)$ which are isospectral to the original potential $U_1(z)$. Their shapes are controlled via the scalar parameter(s) λ_i, which therefore influence the wave functions and the values of various matrix elements while the resonant conditions, once obtained for $U_1(z)$, remain intact.

Here we shall give a brief description of SUSYQM backgrounds and the working formulas. Consider the original potential $U_1(z)$, the eigenfunctions ψ_{1_n}, and eigenenergies E_n, which are all known. One may then construct its partner potential $U_2(z)=U_1(z)-(\hbar^2/m)(d^2/dz^2)\ln\psi_{1_i}$, which has all eigenenergies identical to those of $U_1(z)$, except E_i, which is ''deleted.'' However, the function $1/\psi_{1_i}$ is a solution of the Schrödinger equation with $U_2(z)$ and E_i, and another linearly independent solution is $\int_{-\infty}^{z}\psi_{1_i}^2(z')dz'/\psi_{1_i}$, so the general solution may be written as

$$\psi_{2_i}(\lambda_i)=(\lambda_i+I_i)/\psi_{1_i}, \tag{6}$$

where $I_i=\int_{-\infty}^{z}\psi_{1_i}^2(z')dz'$, and λ_i is a parameter that may take any value out of the interval $-1\leqslant\lambda_i\leqslant0$. SUSYQM then enables one to restore the state at $E=E_i$ by setting the potential $U_1(z)-(\hbar^2/m)(d^2/dz^2)[\ln(I_i+\lambda_i)]$, which is thus fully isospectral to the original potential, and depends on the parameter λ_i (i.e., a single-parameter family of isospectral potentials is thus defined).

Instead of immediately restoring the $E=E_i$ state, however, one may choose to delete one more state of $U_1(z)$, i.e., having found $U_2(z)$ its partner potential $U_3(z)=$

$U_2(z)-(\hbar^2/m)(d^2/dz^2)\ln\psi_{2_j}$, which is isospectral to $U_2(z)$ except that the state at $E=E_j$ is missing. The general solution of the Schrödinger equation for this energy is $\psi_{3_j}(\lambda_j)=(I_j+\lambda_j)/\psi_{2_j}$, where $I_j=\int_{-\infty}^{z}\psi_{2_j}^2(z')dz'$, and λ_j is a new parameter. The solution corresponding to some state l is obtained by using the operator $\hat{A}_2=(d/dz)-[\ln(\psi_{2_j})]'$, i.e., $\psi_{3_l}=\hat{A}_2\psi_{2_l}(\lambda_i)$. Now, restoring the state j delivers the new potential $U_4(z)=U_2(z)-(\hbar^2/m)(d^2/dz^2)\{\ln[\lambda_j+I_j(z)]\}$, which is isospectral to $U_2(z)$, its eigenfunctions being given by $\psi_{4_j}=1/\psi_{3_j}$ and $\psi_{4_l}=\hat{A}_2^+\psi_{3_l}$, where $\hat{A}_2^+=-d/dz+[\ln(\psi_{3_j})]'$. The final step is to restore the state i, from which the two-parameter family of potentials is obtained:

$$U_{5_{SS}}(\lambda_i,\lambda_j)=U_1-\frac{\hbar^2}{m}\frac{d^2}{dz^2}\ln[\psi_{1_i}(\lambda_j+I_j)\psi_{4_i}],$$

$$\lambda_{i,j}<-1\vee\lambda_{i,j}>0, \tag{7}$$

which is fully isospectral to $U_1(z)$. The wave functions corresponding to it are given by

$$\psi_{5_i}=1/\psi_{4_i},$$

$$\psi_{5_k}=-\frac{d}{dz}\psi_{4_k}+(\ln\psi_{4_i})'\psi_{4_k},\quad (k\neq i). \tag{8}$$

The procedure may be extended in the obvious manner to introduce more parameters.[5] An alternative approach would be to start with an original potential, delete and immediately restore one of its states i, which delivers the single parameter dependent family $U_{SS}(\lambda,z)=U_1(z)-(\hbar^2/m)(d^2/dz^2)[\ln(\lambda+I(\lambda)]$, and its eigenfunctions

$$\psi_{SS_i}=\frac{\sqrt{\lambda(\lambda+1)}}{\lambda+I(z)}\psi_{1_i}(z),$$

$$\psi_{SS_k}=\psi_{1_k}-\frac{\varphi(z)}{\lambda+I(z))}\int_{-\infty}^{z}\varphi(z')\psi_{1_k}(z')dz',\quad (k\neq i), \tag{9}$$

where $I(z)=\int_{-\infty}^{z}\varphi^2(z')dz'$, and $\varphi(z)$ is the eigenfunction of (arbitrarily chosen) lth state of the original potential.

This procedure should then be repeated taking the current U_{SS} as the new original, and the sequence of SUSYQM transforms $U_1(z)\rightarrow U_{SS}(\lambda_i,z)\rightarrow U_{SS}(\lambda_i,\lambda_j,z)\rightarrow\cdots$ introduces an additional free parameter (λ_l, which is continuously variable) and a discrete parameter (l, the state in respect to which the transformation is made) per each new transform.

The SUSYQM theory is normally used for the constant (effective) mass system. This may represent a drawback for its application to semiconductor quantum-well systems, because the effective mass there will almost certainly be variable.[6–8] In particular, in QW's based upon graded ternary alloys $A_xB_{1-x}C$, the potential and the effective mass are related via $U(z)=[\Delta E_c/\Delta m]m(z)\equiv\theta m(z)$, where ΔE_c is the conduction-band offset between AC and BC materials, and Δm is the difference of electron effective masses in them. It is therefore impossible to realize, by grading a ternary alloy, the constant-mass-variable-potential Hamiltonian, as delivered by SUSYQM.

There is, however, a remedy to this situation, which relies on using the coordinate transform. The idea is to map the real space, with variable-mass Hamiltonian, into a space where the mass would appear to be constant, and apply the SUSYQM in this latter space. In effect, we introduce an (invertible) coordinate transform $z=g(y)$ into the Schrödinger equation,[6,7] [note that $U(z)=\theta m(z)$, as appropriate for ternary alloy]:

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m(z)}\frac{d\Psi}{dz}\right)+\theta m(z)\Psi=E\Psi, \tag{10}$$

so it becomes

$$\frac{d^2\underline{\psi}}{dy^2}-\frac{d}{dy}[\ln(\underline{m}g')]\frac{d\underline{\psi}}{dy}-\frac{2(\underline{m}g')^2}{\hbar^2}[\theta\underline{m}-E]\underline{\psi}=0, \tag{11}$$

where $\underline{m}(y)=m(g(y)),\underline{\psi}=\psi(g(y)),g'\equiv[dg(y)]/dy$. Defining the scaled wave functions as

$$\underline{\psi}=u(y)\sqrt{\underline{m}g'} \tag{12}$$

the term in front of $d\underline{\psi}/dy$ in Eq. (11) becomes zero, and this equation reads[6]

$$\frac{d^2u}{dy^2}+\left[A(y)-\frac{2\underline{m}g'^2}{\hbar^2}[\theta\underline{m}-E]\right]u=0,$$

$$A(y)=-\frac{1}{4}\left(\frac{1}{\underline{m}g'}\frac{d(\underline{m}g')}{dy}\right)^2+\frac{1}{2}\frac{d}{dy}\left(\frac{1}{\underline{m}g'}\frac{d(\underline{m}g')}{dy}\right). \tag{13}$$

This last expression takes the standard Schrödinger form if the coordinate transform function g satisfies

$$\underline{m}g'^2=m^*>0, \tag{14}$$

$$A(y)-\frac{2\underline{m}g'^2}{\hbar^2}\theta\underline{m}=-\frac{2\underline{m}g'^2}{\hbar^2}U_0(y), \tag{15}$$

where m^* is independent on z, and $U_0(y)$ is any (suitable) function, specified in advance. The spectra of Eq. (10) and (13) are clearly identical, and it is generally advantageous to choose $U_0(y)$, with the constant mass m^*, so that its eigenenergies and eigenfunctions are explicitly known. In the problem considered here, these are chosen to be the output of the SUSYQM method, as described in the previous section, therefore the spectrum of $U(z)$ is as desired, and the wave functions $\psi(z)$, in real space, will become uniquely and straightforwardly [via Eq. (12)] determined once the function $g(y)$ or, equivalently, $m(z)$ is known.

In order to find $m(z)$ we introduce a new function $v(y)$ and substitute $\underline{m}=1/[4qm_0\theta v^2]$ in Eqs. (14) and (15), where $q=2m_e/\hbar^2$ and $m_0=m^*/m_e$ (here m_e denotes the free-electron mass), which results in the nonlinear differential equation

$$2vv''-v'^2-4qm_0U_0(y)v^2+1=0. \tag{16}$$

Its solutions may be written[9] as $v(y)=s_1 s_2$, where s_1 and s_2 are two solutions of the characteristic equation

$$s''-qm_0U_0(y)s=0 \tag{17}$$

chosen so that their Wronskian satisfies $[W(s_1,s_2)]^2=1$. In order to find $s_{1,2}$ we take that the potential U_0 may be written as

$$U_0(y)\equiv v_0(y)+V_0, \quad v_0(y)=\begin{cases} f(y)<0, & |y|<y_{max}, \\ 0, & |y|\geqslant y_{max}, \end{cases} \tag{18}$$

where V_0 is a positive constant which determines the asymptotic value of $m(y)$, and $2y_{max}$ is the range where the potential varies significantly enough, before taking a constant value V_0. Now we write the two particular solutions $s_{L,R}$ in the form

$$s_L(y)=\begin{cases} e^{-ky}+R_L e^{ky}, & y\leqslant -y_{max}, \\ A_L g_1(y)+B_L g_2(y), & |y|<y_{max}, \\ T_L e^{-ky}, & y\geqslant y_{max}, \end{cases} \tag{19}$$

$$s_R(y)=\begin{cases} T_R e^{ky}, & y\leqslant -y_{max}, \\ A_R g_1(y)+B_R g_2(y), & |y|<y_{max}, \\ R_R e^{-ky}+e^{ky}, & y\geqslant y_{max}, \end{cases} \tag{20}$$

where $k=\sqrt{qm_0V_0}$, and the functions $g_{1,2}$ satisfy the fundamental boundary conditions at $y=0$, i.e., $g_1(0)=1$, $g_1'(0)=1$, $g_2(0)=0$, $g_2'(0)=1$. The solutions $s_{L,R}$ should be multiplied by a suitable constant C to get $s_{1,2}$ that satisfy $[W(s_1,s_2)]^2=1$, and in terms of which the solution to the original problem reads

$$\underline{m}(y)=\frac{1}{4qm_0\theta[C_1 s_1^2\pm\sqrt{1+4C_1C_2}s_1s_2+C_2{s_2}^2]^2}, \tag{21}$$

where $C_{1,2}$ are some constants. From the equality of Wronskians at $y=\pm y_{max}$ it follows $T_L=T_R=T$, and the value of ''normalization'' constant C is then straightforwardly found, so Eq. (21) becomes

$$\underline{m}(y)=\frac{(V_0/\theta)T^2}{[C_1 s_L^2\pm\sqrt{1+4C_1C_2}s_Ls_R+C_2s_R^2]^2}. \tag{22}$$

If $\underline{m}(y)$ is to remain nonzero at $y=\pm\infty$ we must set $C_1=0$ and $C_2=0$. Finally, the constants $A_{L,R}$, $B_{L,R}$, $R_{L,R}$, and T are determined from the continuity of $s_{L,R}$ and $s_{L,R}'$ at $\pm y_{max}$, and the effective mass vs coordinate dependence reads

$$\underline{m}(y)=\begin{cases} \dfrac{V_0/\theta}{[1+R_Le^{2ky}]^2}, & y\leqslant -y_{max}, \\ \dfrac{(V_0/\theta)T^2}{\{[A_Rg_1(y)+B_Rg_2(y)][A_Lg_1(y)+B_Lg_2(y)]\}^2}, & |y|<y_{max}, \\ \dfrac{V_0/\theta}{[1+R_Re^{-2ky}]^2}, & y\geqslant y_{max}. \end{cases} \tag{23}$$

The normalized wave functions in real space are given in parametric form as

$$\underline{\psi}=u(y)\frac{\sqrt[4]{\underline{m}(y)}}{\sqrt[4]{m_0}},$$

$$z=g(y)=\sqrt{m_0}\int_{y_0}^{y}\frac{dy'}{\sqrt{\underline{m}(y')}} \tag{24}$$

and correspond to the potential in real space $U(z)=\theta m(z)$, realizable by graded ternary alloy.

III. NUMERICAL RESULTS

In the optimization of QW shape, to get maximal electro-optic effect, we started with symmetric Pöschl-Teller potential,[10,11]

$$U(y)=-\frac{\tilde{U}}{\cosh^2(y/d)}. \tag{25}$$

Its energies are known analytically, as $E_i=-(\hbar^2/8m^*d^2)\{-(1+2i)+[1+(8\tilde{U}d^2m^*/\hbar^2)]^{1/2}\}^2$, $i=0,1,2,\ldots,$ and for any value of the parameter $\tilde{U}$ one may find the half-width d, which provides the appropriate spacing of the two lowest states, $(E_{10}=E_1-E_0)$. The bound-state wave functions for this potential are also known explicitly: $\psi_0(y)=1/[\cosh(y/d)]^s$, $\psi_1(y)=\sinh(y/d)/[\cosh(y/d)]^s$, $\psi_2(y)=[1+2(1-s)\sinh^2(y/d)]/[\cosh(y/d)]^s,\ldots,$ where $s=1/2\{-1+[1+(8\tilde{U}m^*d^2/\hbar^2)]^{1/2}\}$, (Ref. 10). Taking this potential as the original, we made the SUSYQM transform of deleting and restoring the lowest two states, which delivered the potential dependent on two parameters, $v_0(\lambda_i,\lambda_j,y)$, i.e., the potential $U_0=v_0+V_0$ with analytically known eigenvalues and eigenfunctions. Then, using the coordinate transform method, we constructed the variable-mass-variable-potential Hamiltonian, with $U(\lambda_i,\lambda_j,z)=U^*(\lambda_i,\lambda_j,z)+V_0$

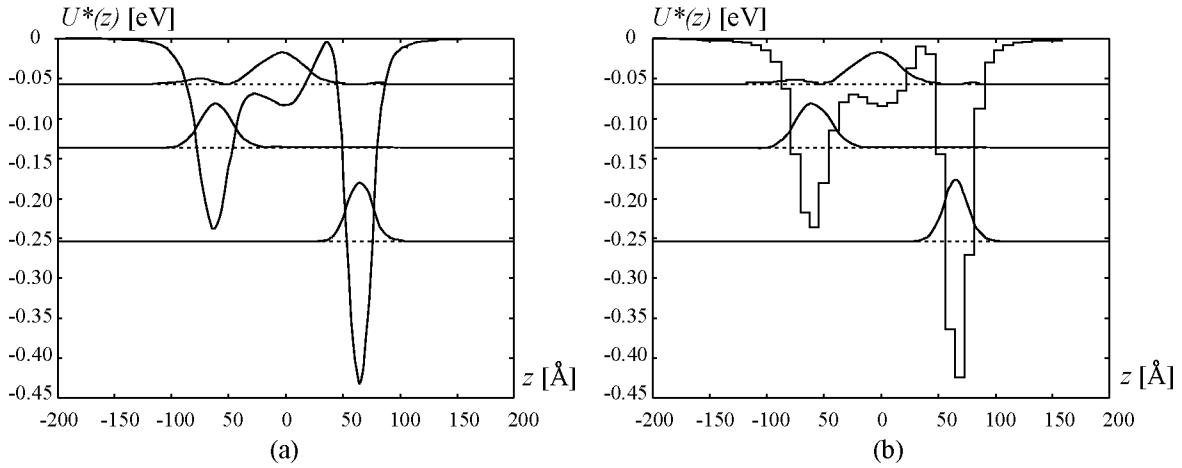

FIG. 1. (a) The optimum QW potential shape, and the envelope wave functions squared, calculated when maximizing the Stark effect derived susceptibility, and (b) the discretized, step-graded, version of this potential, with the step width equal to three crystalline monolayers.

$=\theta m(\lambda_i,\lambda_j,z)$. By varying the parameters λ_i and λ_j we found widely changing values of dipole matrix elements between relevant states. For some values of λ_i and λ_j, one or another component of the second-order susceptibility (4) becomes highly dominant.

In numerical calculations we used the values $m^*=0.075m_e$, $\tilde{U}=0.32$ eV, $E_{10}=116$ meV, $V_0=1.265$ eV, $\theta=9.036$ (in eV/m_e units), which enable the realization of the obtained potential by $Al_xGa_{1-x}As$ alloy (the value of V_0 was chosen so that the effective mass never exceeds 0.15 m_e, i.e., the largest possible value in this alloy). Furthermore, the conduction band offset was $\Delta E_c=750$ meV, and $m_{GaAs}=0.067m_e$, $m_{AlAs}=0.15m_e$. The functions $s_{L,R}$, which determine the effective mass dependence (23), were calculated by the fourth- or fifth-order Runge-Kutta method, combined with a modification of the WBK method. With the Pöschl-Teller potential depth of $\tilde{U}=0.32$ eV, the appropriate value of $d=53.67$ Å will deliver the required $E_{10}=116$ meV, and such potential supports four bound states, with $E_0=-253.2$, $E_1=-137.2$, $E_2=-56.5$, and $E_3=-11.0$ meV.

The (λ_i,λ_j) parameters space was first searched for the largest value of Stark susceptibility. The maximum value was found for $\lambda_i=-1.0002$, $\lambda_j=0.01$, and the corresponding QW profile is displayed in Fig. 1(a). This structure has $M_{13}\approx 0$ and $|M_{22}-M_{11}|=125.9$ Å. Certainly, the continuous grading (i.e., potential) is not exactly realizable, and in Fig. 1(b) we give the discretized step-graded version of the optimized QW profile, with the step width of 3×2.83 Å (3 ML). This discretization changes the energies and matrix elements insignificantly, i.e., to $E_0=-253.2$ meV, $E_1=-137.8$ meV, $E_2=-55.0$ meV, $M_{13}=0.29$ Å, $|M_{22}-M_{11}|=125.8$ Å. For comparison, we note that a QW for this type of electro-optic effect was designed in Ref. 1. Unfortunately, neither the values of matrix elements obtained, nor the materials parameters used in calculation, were stated therein. So, using the same parameters as in this work, we could estimate that the QW of Fig. 1 provides $|M_{22}-M_{11}|\approx 20$ Å (indeed, it is not claimed that this QW has been optimized in any way), and the design presented here is significantly better.

Another search was performed to find the best QW shape for the type-II QI effect. Here we seek for the structure with $M_{22}-M_{11}=0$ while $M_{13}\neq 0$ and as large as possible. The best result obtained was $M_{13}=2.58$ Å and $M_{22}-M_{11}\approx 0$, which occurs with the values of SUSYQM parameters $\lambda_i=0.0197$ and $\lambda_j=0.1$. The optimized potential shape and its discretized version are given in Figs. 2(a) and 2(b). Here again the discretization produces only minor changes in re-

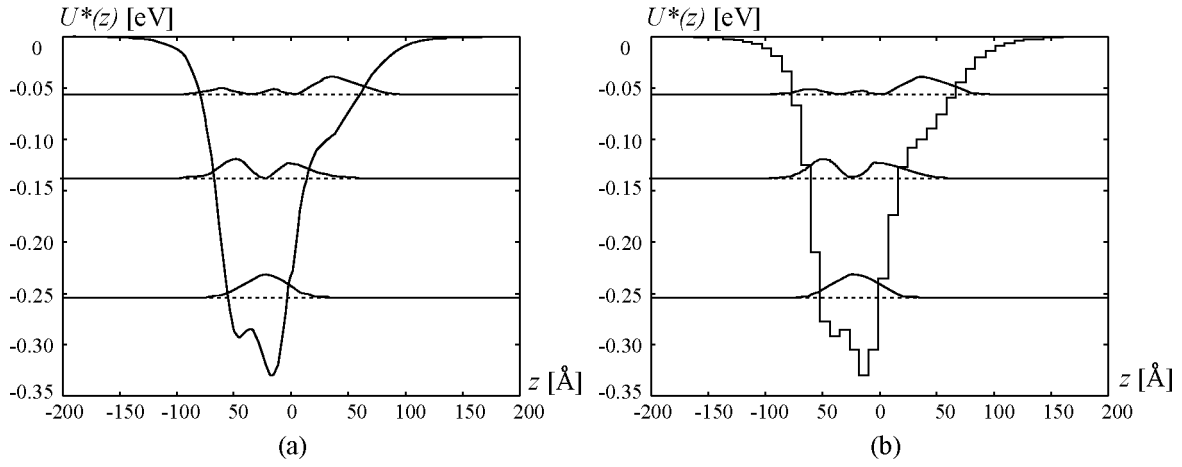

FIG. 2. Same as Fig. 1, but for maximizing the type-II quantum interference derived susceptibility.

sults, i.e., $E_0=-253.0$ eV, $E_2=-136.6$ eV, $E_3=-55.2$ eV, $M_{22}-M_{11}=0.013$ Å, $M_{13}=2.38$ Å. A QW designed for this type of electro-optic effect was presented in Ref. 3, for which we could estimate the value $|M_{13}|\approx 0.675$ Å (it is not explicitly stated therein), and the design presented here is again significantly better.

IV. CONCLUSION

A method is described for the optimized design of quantum-well structures with respect to the second-order susceptibilities relevant for electro-optic applications. The method relies on isospectral transformations (SUSYQM and coordinate transform). It starts by some initial potential, which may even be symmetric, to generate a family of potentials, the shape of which is controlled by one or more scalar parameters, and which are accompanied with the effective mass variation proportional to the potential variation, being therefore realizable in graded ternary alloys. By varying the values of control parameters, i.e., the potential shape, one can change the values of dipole matrix elements relevant for a particular susceptibility, and find the best potential shape, while the energy levels, once obtained in the initial potential, remain unchanged throughout this search. In this work the optimized potentials have been found for either the linear Stark effect derived or for quantum interference derived electro-optical effects.

There are numerous possible generalizations and modifications of the procedure used in this work. Using the initial potential other than Pöschl-Teller (possibly asymmetric), choosing the states for the SUSYQM transform other than the lowest two, introducing more free parameters—these may improve the results of the optimization, though it is difficult to assess the potential benefits from all these directions, either theoretically or by numerical experimenting.

*Electronic address: milanovic@kiklop.etf.bg.ac.yu

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