



## Supersymmetric quantum-well shape optimization for intersubband bound–continuum second harmonic generation

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A method is described for the optimized design of quantum-well structures, with respect to maximizing the second-order susceptibilities relevant for second harmonic generation. The possibility is explored of obtaining resonantly enhanced nonlinear optical susceptibilities in quantum wells with two bound states and a continuum resonance state as the dominant third state. The method relies on applying the isospectral (energy structure preserving) transformations to an initial Hamiltonian in order to generate a parameter-controlled family of Hamiltonians. By changing the values of control parameters one changes the potential shape and thus the values of matrix elements relevant to susceptibility to be maximized. The method was used for the design of  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -based QWs. The results indicate the possibility of employing continuum states in resonant second harmonic generation at higher photon energies,  $\hbar\omega = 200\text{--}300$  meV.

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### 1. Introduction

Bandgap engineering of semiconductor quantum-well (QW) structures has been employed for optimizing the performance of various QW-based devices [1]. By varying the structure profile, the quantized states' energies and wavefunctions may be tailored, so as to best suit a particular application. In particular, there has been an increasing interest in nonlinear optical effects based on intersubband transitions between quantized states in asymmetric QWs [2–17]. Large transition matrix elements ( $\sim\text{nm}$ ) and the possibility of achieving resonance conditions (subsequent level spacing equal to the pump photon energy), which greatly enhance the nonlinearity are advantages of using those structures for second harmonic generation (SHG). It was a common practice to take all three states needed for SHG to be bound, and various QWs were analyzed for this case, e.g. compositionally graded, in a stepwise-constant manner, step QWs [3–7], electric-field-biased QWs [8, 9] and asymmetric-coupled QWs [10–12]. Recently, some research effort has been put into finding the best potential shape of continuously graded QWs [13–16]. However, most of the papers published so far describe resonant SHG for the pump photon energy value of  $\hbar\omega = 116$  meV, which corresponds to  $\text{CO}_2$  laser input [3–16] or even larger wavelengths [17]. The reason is that for this pump photon energy it is relatively straightforward to achieve conditions necessary for SHG in common  $\text{GaAs}/\text{Al}_x\text{Ga}_{1-x}\text{As}$ -based

QWs. It becomes difficult or impossible to a QW with three bound states, for pump photon energies much higher than 116 meV. States above the barrier, for this application, may be favorable as the third state.

For a specified pump photon energy the QW shape may be designed to provide the most efficient second harmonic generation, i.e. the largest value of the corresponding second-order susceptibility which describes nonlinear polarization at twice the frequency of the pump field. In this paper, we discuss a systematic method of optimizing the smooth potential shape (profile) and explore the possibility of using QWs with two bound states and a free state above the barrier for higher energy intersubband SHG in continuously graded ternary-alloy-based QWs. One can imagine such a QW approximately comprises a large number ( $\sim 10^2$ ) of thin layers with constant composition (there is some justification for this, both from a technological viewpoint and due to the fact that composition variation within one lattice constant is meaningless). Setting up the procedure for such a system, and performing the (essentially global) optimization would be highly impractical; solving a large system of nonlinear equations is extremely time consuming and potentially unsuccessful unless a good initial guess is provided.

The method of optimizing the QW potential shape used in this paper relies on theoretical tools of supersymmetric quantum mechanics (SUSYQM) [18]. This will first be described in Section 2 and its use will be illustrated in Section 3. Single-parameter-dependent isospectral transformation of an initial potential will be used to generate a class of asymmetric potentials. The method is systematic in the sense that all potentials of a given class are explored, i.e. no potential better than that found as optimal may exist in that class.

Calculations were performed for GaAs/AlGaAs-based QWs which, using the bound–continuum transitions, enable higher energy ( $\hbar\omega = 200\text{--}300$  meV) intersubband resonant SHG.

## 2. Theoretical consideration

### 2.1. Second-order susceptibility

We consider an n-doped QW structure based on a direct bandgap semiconductor. The bandgap throughout such a structure should be large enough that interband transitions may be neglected. Nonlinear polarization at twice the frequency of the pump field, acting as the source of the second harmonic field, is described by the second-order susceptibility  $\chi^{(2)}$ . The polarization response of the structure to the pump field with photon energy  $\hbar\omega$  is mainly governed by intersubband transitions between quantized (bound or continuum) conduction band states  $E_i$ . Under those conditions the second-order susceptibility  $\chi^{(2)}$  is significant only for the pump and harmonic field polarized perpendicular to the QW plane ( $z$ -axis), i.e.  $\chi^{(2)} = \chi_{zzz}^{(2)}$ . It is given by the general expression (e.g. [5]):

$$\chi_{zzz}^{(2)} = \frac{e^3}{L_z \epsilon_0} \sum_i \sum_j \frac{1}{(2\hbar\omega - \Delta E_{ji}) - i\hbar\Gamma_{ji}} \times \sum_l M_{ij} M_{jl} M_{li} \left[ \frac{\rho_{ii} - \rho_{ll}}{\hbar\omega + \Delta E_{li} - i\hbar\Gamma_{li}} - \frac{\rho_{ll} - \rho_{jj}}{\hbar\omega - \Delta E_{jl} - i\hbar\Gamma_{jl}} \right], \quad (1)$$

where  $M_{ij} = \langle \Psi_i | z | \Psi_j \rangle$  are the transition dipole matrix elements,  $\Delta E_{ij}$  the transition energies between states  $i$  and  $j$ ,  $\rho_{ii}$  denotes the electron sheet density corresponding to state  $i$ , (summation over 2D in-plane wavevectors is already performed in eqn (1), so the sheet densities  $\rho_{ii}$  appear therein),  $\Gamma_{ij}$  the off-diagonal relaxation rates and  $L_z$  the length of structure. In the majority of feasible structures almost all electrons normally reside in the lowest state (i.e.  $\rho_{ii} \ll \rho_{00}$  for  $i > 0$ ).

In the case of having continuum (free) states contributing to the process, we consider the asymmetric QW with two bound states (with energies  $E_0$  and  $E_1$ ) and continuum states  $E_{\text{cont}}$  ( $E_{\text{cont}} > 0$ ). The energy of the continuum states is described by the perpendicular (to the QW plane) wavevector  $k_B$  in the barrier region, i.e.  $E_{\text{cont}}(k_B) = \hbar^2 k_B^2 / 2m_B$ , where  $m_B$  is the effective mass in the barrier. Continuum states will hereafter

be labeled with the subscript  $k_B$ . Owing to the denominators with energy differences, the expression for  $\chi_{zzz}^{(2)}$  grossly simplifies under the resonance conditions, i.e. when some of the states are spaced by about the ‘pump’ photon energy  $\hbar\omega$ , with just one term with these ‘properly spaced’ states remaining as important (resonantly enhanced). We hold that only the ground state is significantly populated with electrons, and the QW is tailored such that the two bound states are spaced by exactly the pump photon energy. The summation in eqn (1) is performed over all continuum states. Wavefunctions corresponding to the states above the barrier are normalized by using the box-boundary conditions. If  $M_{01}$  is the bound–bound matrix element, and  $\hat{M}_{0k_B}$  and  $\hat{M}_{1k_B}$  represent matrix elements calculated with non-normalized above-the-barrier state real wavefunctions and normalized bound state (0 or 1) wavefunctions, the real part of  $\chi_{zzz}^{(2)}$ , which is of interest to us, may be written as:

$$\chi_{zzz}^{(2)} = \frac{e^3}{L_z \epsilon_0} \rho_{00} M_{01} \frac{1}{L_z} \sum_{k_B} \frac{\hat{M}_{0k_B} \hat{M}_{1k_B}}{(\hbar\Gamma)^2 + [(2\hbar\omega) - (E_{k_B} - E_0)]^2} \frac{\Delta k_B}{\Delta k_B}. \quad (2)$$

Here we take  $\Gamma_{01} = \Gamma_{0k_B} = \Gamma_{1k_B} = \Gamma$  (the linewidth  $\hbar\Gamma$  is taken to be common to all transitions, as is often assumed for bound states in the literature). In fact, this is not quite true: the electron-scattering-induced part of the linewidth may be significantly different, but within the order of magnitude, for various transitions. However, transitions to continuum states have another component of the linewidth, stemming from the width of the resonance, and it always dominates other sources of broadening. In particular, for the QWs treated in this work we find the resonance widths to be  $\geq 30$  meV, when we used the value  $\hbar\Gamma = 5$  meV, so it is clear that doubling or even tripling this latter value would not change the final result too much. The matrix elements with states belonging to the continuum need to be calculated twice, because of the double degeneracy (i.e. with both wavefunctions corresponding to energy  $E_{k_B}$ ). These two wavefunctions should be taken in the form of scattering states (i.e. to be orthogonal), which prevents under or over completeness in summing over all continuum states in eqn (2). In the full continuum limit:  $L_z \rightarrow +\infty$ ,  $\Delta k_B \rightarrow dk_B$  and  $\sum \rightarrow \int$ , and with  $\Delta k_B = \pi/L_z$  eqn (2) becomes

$$\chi_{zzz}^{(2)} = \frac{e^3 \rho_{00} M_{01}}{L_z \epsilon_0 \pi} \int_{(k_B)} \frac{\hat{M}_{0k_B}(E_0, E_{k_B}) \hat{M}_{1k_B}(E_1, E_{k_B})}{(\hbar\Gamma)^2 + [(2\hbar\omega) - (E_{k_B} - E_0)]^2} dk_B \equiv \frac{e^3}{L_z \epsilon_0} \rho_{00} \Pi^*. \quad (3)$$

In QWs with two bound states’ wavefunctions localized in the well, one expects that the continuum state wavefunctions close to the resonances will give the largest contribution in eqn (3), because of the largest bound–continuum matrix elements. The contribution of resonance states is particularly enhanced at photon energies for which  $E_{k_B} - E_0 \approx 2\hbar\omega$ , as follows from the denominator of eqn (3). For these two reasons, the largest  $\chi^{(2)}$  is to be expected with double resonance achieved with the two bound and a resonance state, i.e.  $E_{k_B} - E_0 = E_{\text{res}} - E_0 = 2(E_1 - E_0) = 2\hbar\omega$ .

## 2.2. Isospectral transformation of the potential

In order to optimize the QW shape with respect to the second-order susceptibility, one may vary the shape (and hence the wavefunctions) subject to the constraint that spacings between the relevant states remain unchanged, and look for the value of susceptibility (i.e. parameter  $\Pi^*$ ), which depends on the the QW shape (via the dipole matrix elements). In the case of  $\chi^{(2)}$ , because of definite parity of wavefunctions, symmetric QWs are ruled out, so one should consider asymmetric structures only. The 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) [18]. Starting from an initial (‘original’) potential for which it was achieved, in whatever way, that its quantized states’ energies or their spacing are as required, this technique allows one to generate a family of parameter-dependent potentials which are all isospectral to the original.

Here we shall give a brief description of the working SUSYQM formulas. Consider the original potential

$U(z)$ , with constant mass, for which eigenfunctions  $\Psi_n$  and eigenenergies  $E_n$  are all known. The supersymmetric partner potential  $U_{SS}(\lambda, z)$ , isospectral to the original  $U(z)$ , is given by

$$U_{SS}(\lambda, z) = U(z) - \frac{\hbar^2}{m} \frac{d^2}{dz^2} [\ln(\lambda + I(z))], \quad (4)$$

and normalized eigenfunctions corresponding to  $U_{SS}(\lambda, z)$  are related to those of the original, via

$$\Psi_{SS_i}(z) = \Psi_i(z) + \frac{\varphi(z)}{\lambda + I(z)} \int_z^{+\infty} \varphi(t) \Psi_i(t) dt, \quad (5)$$

where  $\Psi_i(z)$  is the eigenfunction of the  $i$ th state,  $\varphi(z)$  denotes any other bound state of the original potential, and

$$I(z) = \int_{-\infty}^z \varphi^2(t) dt. \quad (6)$$

Specifically, choosing  $\varphi(z) = \Psi_l(z)$ , i.e. the  $l$ th state as the factorization state, all the transformed wavefunctions for states  $i \neq l$  are given by (5), and the one corresponding to  $i = l$  by

$$\Psi_{SS_l}(z) = \frac{\sqrt{\lambda(\lambda + 1)}}{\lambda + I(z)} \Psi_l(z). \quad (7)$$

The free scalar parameter  $\lambda$  in eqns (4)–(7) may take any value except those in the range  $-1 \leq \lambda \leq 0$ . In the special case of symmetric original potential it may be shown that  $U_{SS}(z, \lambda) = U_{SS}(z, -(\lambda + 1))$ , so all physically different  $U_{SS}(\lambda, z)$  may be obtained with positive  $\lambda$  only. This procedure generates a single-parameter-dependent family of potentials and corresponding wavefunctions, while subsequent application of SUSYQM transform would introduce more parameters, i.e.  $U_{SS}(z) \rightarrow U_{SS}(\lambda, z) \rightarrow U_{SS}(\lambda, \mu, z) \rightarrow \dots$ . The potential is thus varied continuously through the variation of the parameter  $\lambda$  (more parameters, if introduced), and the evaluation of wavefunctions and matrix elements will then readily deliver the best potential shape.

Along with the continuously variable parameter(s) that control the shape of the partner potential, there is an additional discrete parameter—the factorization state index  $l$ , which adds more freedom. It is important to note, however, that it is the original potential that determines the set of potentials which can be derived from it. Therefore, the SUSYQM-based optimization procedure is not global, but within the class of potentials derived from the chosen original.

The SUSYQM theory is normally used for the constant (effective) mass systems. This prevents its application to semiconductor quantum-well systems. In particular, in QWs based upon graded ternary alloys (i.e.  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ ), the potential and the effective mass are related via  $U(z) = [\Delta E_c / \Delta m] m(z) \equiv \theta m(z)$ , where  $\Delta E_c$  is the conduction band offset between materials and  $\Delta m$  is the difference of electron effective masses in them. There is a solution to this problem, if we introduce an invertible coordinate transformation  $z = g(y)$  into the Schrödinger equation:

$$-\frac{\hbar^2}{2} \frac{d}{dz} \left( \frac{1}{m(z)} \frac{d\Psi}{dz} \right) + U(z)\Psi = E\Psi, \quad (8)$$

so it becomes:

$$\frac{d^2 \underline{\Psi}}{dy^2} - \frac{d}{dy} [\ln(\underline{m}g')] \frac{d\underline{\Psi}}{dy} - \frac{2(\underline{m}g')^2}{\hbar^2} [\theta \underline{m} - E] \underline{\Psi} = 0, \quad (9)$$

where  $\underline{m}(y) = m(g(y))$ ,  $\underline{\Psi} = \Psi(g(y))$ ,  $g' \equiv \frac{dg(y)}{dy}$ . Defining the scaled wavefunctions as

$$\underline{\Psi} = u(y) \sqrt{\underline{m}g'}. \quad (10)$$

Equation (9) takes the standard Schrödinger form if the coordinate transform function  $g$  satisfies the condition  $\underline{m}g'^2 = m^* > 0$ , where  $m^*$  is independent on  $z$ :

$$\frac{d^2u}{dy^2} - \frac{2\underline{m}g'^2}{\hbar^2} \left[ \theta \underline{m} + \frac{\hbar^2}{8\underline{m}g'^2} \left( \frac{1}{\underline{m}g'} \frac{d(\underline{m}g')}{dy} \right)^2 - \frac{\hbar^2}{4\underline{m}g'^2} \frac{d}{dy} \left( \frac{1}{\underline{m}g'} \frac{d(\underline{m}g')}{dy} \right) - E \right] u = 0. \quad (11)$$

The spectra of eqns (8) and (11) are clearly identical. Here we can introduce  $U_0(y)$ , with the constant mass  $m^*$  so that its eigenenergies and eigenfunctions are explicitly known.

In order to find  $m(z)$  we introduce a new function  $v(y)$  and substitute  $m = 1/[4qm_0\theta v^2]$  in eqn (11), 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

$$2vv'' - v'^2 - 4qm_0U_0(y)v^2 + 1 = 0. \quad (12)$$

Its solution may be written as  $v(y) = s_1s_2$ , where  $s_1$  and  $s_2$  are two solutions of the characteristic equation

$$s'' - qm_0U_0(y)s = 0, \quad (13)$$

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

$$U_0(y) = v_0(y) + V_0, \quad v_0(y) = \begin{cases} f(y) < 0, & |y| < y_{\max} \\ 0, & |y| \geq y_{\max}, \end{cases} \quad (14)$$

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

$$s_L(y) = \begin{cases} e^{-ky} + R_L e^{ky}, & y \leq -y_{\max} \\ A_L g_1(y) + B_L g_2(y), & |y| < y_{\max} \\ T_L e^{-ky}, & y \geq y_{\max} \end{cases} \quad (15)$$

$$s_R(y) = \begin{cases} T_R e^{ky}, & y \leq -y_{\max} \\ A_R g_1(y) + B_R g_2(y), & |y| < y_{\max} \\ R_R e^{-ky} + e^{ky}, & y \geq y_{\max}, \end{cases} \quad (16)$$

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  $[W(s_1, s_2)]^2 = 1$ . From the equality of Wronskians at  $y = \pm y_{\max}$  it follows that  $T_L = T_R = T$ , and the value of the 'normalization' constant  $C$  is easily found. 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 versus coordinate dependence then reads

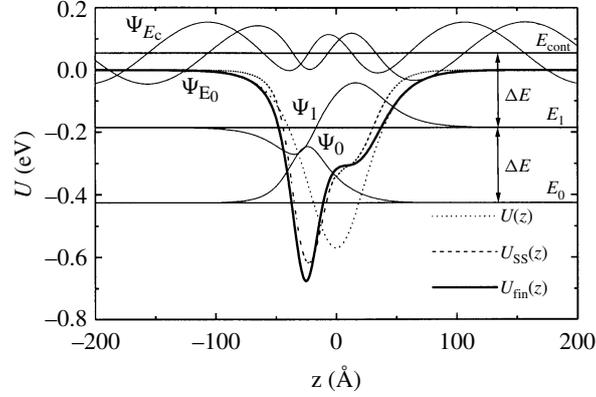
$$\underline{m}(y) = \begin{cases} \frac{V_0/\theta}{[1+R_L e^{2ky}]^2} & y \leq -y_{\max} \\ \frac{(V_0/\theta)T^2}{\{[A_R g_1(y) + B_R g_2(y)][A_L g_1(y) + B_L g_2(y)]\}^2} & |y| < y_{\max} \\ \frac{V_0/\theta}{[1+R_R e^{-2ky}]^2} & y \geq y_{\max}. \end{cases} \quad (17)$$

The normalized wavefunctions in real space are given in parametric form as

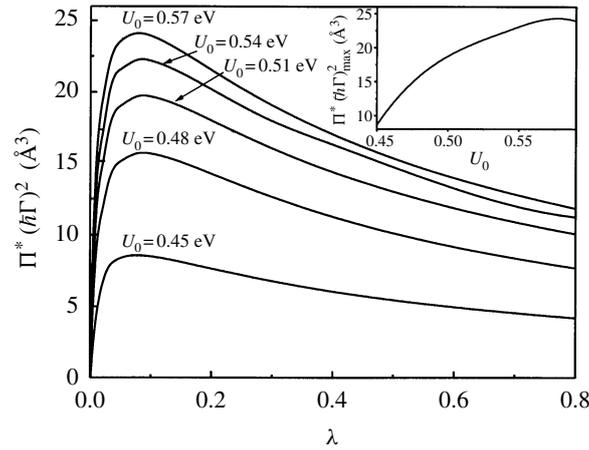
$$\underline{\Psi} = u(y) \frac{\sqrt[4]{\underline{m}(y)}}{\sqrt[4]{m_0}} \quad (18)$$

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

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



**Fig. 1.** The optimized ( $U_0 = 570$  meV,  $\Delta E = 240$  meV,  $\lambda = 0.08$ ) supersymmetric potential  $U_{SS}(z)$  (dashed line), the original  $U(z)$  (dotted line), and final retailed  $U_{fin}(z)$ , the last one to be realized by composition grading of the  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  alloy, providing maximum second-order nonlinear susceptibility.



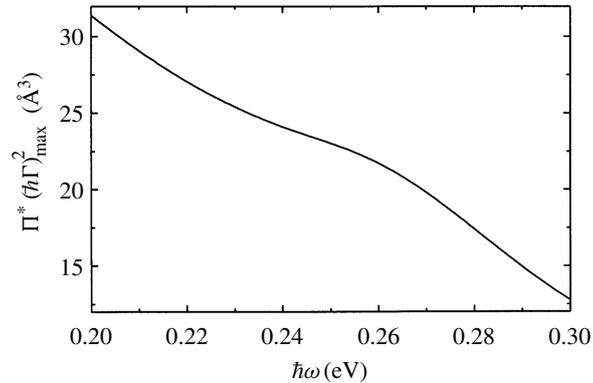
**Fig. 2.** Values of the matrix elements' product  $\Pi^*(\hbar\Gamma)^2$ , obtained with different choices of  $U_0$  and  $\lambda$ . Dependence of the optimized value of  $\Pi^*(\hbar\Gamma)^2$  on  $U_0$  is given in the inset.

### 3. Numerical results and discussion

The optimization procedure was employed for continuously graded ternary alloy QWs, to be used for resonant second harmonic generation of  $\hbar\omega = 240$  meV radiation (this corresponds to a  $5.1 \mu\text{m}$  CO laser, or approximately to a frequency doubled  $\text{CO}_2$  laser used as a pump for the next SHG, or to a quantum cascade laser operating in the mid-infrared [19]). The procedure was then repeated for pump photon energy in the range  $\hbar\omega = 200\text{--}300$  meV. Due to the comparatively large photon energies involved, a technologically favorable  $\text{Al}_x\text{Ga}_{1-x}\text{As}$  alloy does not provide sufficient band offset for classical three bound-state resonant SHG, and the problem was circumvented by introducing bound–continuum transitions.

We have restricted our considerations to the single-parameter-dependent family of potentials, obtained via the SUSYQM transform, from the original Pöschl–Teller potential [20, 21]:

$$U(y) = -\frac{U_0}{\cosh^2(y/d)}. \quad (19)$$



**Fig. 3.** The fully optimized values of  $[\Pi^*(\hbar\Gamma)^2]$  obtainable at various pump photon energies.

Its energies are known analytically as  $E_i = -(\hbar^2/8m^*d^2)\{-1 + 2i + [1 + (8U_0d^2m^*/\hbar^2)]^{1/2}\}^2$ ,  $i = 0, 1, 2, \dots$  and for any value of parameter  $U_0$  one may find the half-width  $d$ , which provides the appropriate spacing of the two lowest states, ( $\Delta E_{10} = E_1 - E_0$ ). The eigenfunctions of bound states for this potential are known explicitly:  $\Psi_0(y) = 1/[\cosh(y/d)]^s$ ,  $\Psi_1(y) = \sinh(y/d)/[\cosh(y/d)]^s$ ,  $\Psi_2(y) = [1 + 2(1-s)\sinh^2(y/d)]/[\cosh(y/d)]^s, \dots$ , where  $s = 1/2(-1 + [1 + (8U_0m^*d^2/\hbar^2)]^{1/2})$  [21]. The free-state wavefunctions are also known, the even function is  $\Psi_{Ee} = F(a, b, c, x)\Psi_0$  and the odd is  $\Psi_{Eo} = x^{1/2}F(a-c+1, b-c+1, 2-c, x)\Psi_0$  where  $F(a, b, c, x)$  is a hypergeometric function,  $x = -\sinh^2(z/d)$ ,  $a = (-s + jkd)/2$ ,  $b = (-s - jkd)/2$ ,  $c = 1/2$ ,  $k = \sqrt{2m^*(E - E_0)/\hbar^2 - (s/d)^2}$ ,  $j = \sqrt{-1}$ , [20]. Taking this potential as the original, we made the SUSYQM transform which delivered the potential dependent on one parameter with analytically known eigenvalues and eigenfunctions. Then, using the coordinate transformation method, we have constructed the variable-mass-variable-potential Hamiltonian (Fig. 1). The material parameters are taken as [22]:  $m_{\text{GaAs}} = m^* = 0.067m_e$ ,  $m_{\text{AlAs}} = 0.15m_e$ ,  $\Delta E_c = 750$  meV,  $\theta = 9.036$  (in  $eV/m_e$  units),  $V_0 = 1.265$  eV and  $\hbar\Gamma = 5$  meV. In the first set of calculations we have found the dependence of the  $\Pi^*$  parameter on  $\lambda$  and  $U_0$ , Fig. 2 (for convenience,  $\Pi^*$  is multiplied by  $(\hbar\Gamma)^2$  to become dimensionally equivalent to the product of matrix elements with all three bound states, i.e.  $[\text{\AA}^3]$ ). The largest value for this set of potentials is  $[\Pi^*(\hbar\Gamma)^2]_{\text{max}} = 24 \text{\AA}^3$  obtained for  $U_0 = 570$  meV and  $\lambda = 0.08$ . For  $\lambda \approx 0.001$  the matrix element between the lowest bound and free state was changed in sign, which indicates that this structure could be used for the design of QW structures with respect to second-order susceptibilities relevant for electro-optic applications, i.e. Stark effect [23]. The procedure was repeated for various values of pump photon energy in the range  $\hbar\omega = 200\text{--}300$  meV. The fully optimized values of  $[\Pi^*(\hbar\Gamma)^2]_{\text{max}}$  are presented in Fig. 3. It is not straightforward to compare this result with those obtained in QWs with all three bound states, because few calculations for this pump photon energy have been done so far. The largest value of the matrix elements' product for 240 meV pump photon energy, in GaN/AlGaIn system with three bound states, amounted to  $\Pi \approx 240 \text{\AA}^3$  [24]. The resonant susceptibility  $\chi^{(2)} \sim \Pi/(\hbar\Gamma)^2$  would be 10 times larger than obtained in this work, but only if the linewidths for all three transitions in a GaN/AlGaIn well are really  $\hbar\Gamma = 5$  meV. Since larger linewidths should be expected for transitions to higher levels, as mentioned above, which will proportionally decrease  $\chi^{(2)}$  in a GaN/AlGaIn QW and only marginally affect  $\chi^{(2)}$  in the QW considered in this paper, we expect the susceptibilities in the two structures to become roughly comparable.

#### 4. Conclusion

A method is described for the optimized design of continuously graded quantum-well structures with respect to higher energy second-order susceptibilities relevant for optical second harmonic generation based on bound–continuum transitions. The method relies on single-parameter-dependent isospectral transformations (SUSYQM and coordinate transformation). By varying the control parameter, i.e. the potential shape, one can change the value of relevant matrix elements and find the best potential shape, while energy levels once obtained in the initial potential remain unchanged throughout this search. The method was applied for optimized design of  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ -based QWs intended for resonant SHG. Similarly, this method could be used for optimization of electro-optic modulation properties in QW structures based on bound–continuum transitions in order to increase the Stark effect.

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