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Quantum well shape tailoring via inverse spectral theory: optimizing resonant second-harmonic generation

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Abstract. A procedure for the design of quantum well structures optimized as regards inter-subband double-resonant second-harmonic generation is proposed. It relies on the inverse spectral theory, allowing one to start from an arbitrary potential and shift its levels to the positions required for a particular application, in this case such that they become equispaced. The free parameters that appear, and determine the shape of the modified potential, are then varied in order to find the optimal potential shape that maximizes the nonlinearity, while level energies are automatically fixed throughout this variation. Furthermore, the procedure is adapted to handle cases of variable effective mass, unlike the conventional inverse spectral theory. The use of this procedure is demonstrated by the designing of a graded AlGaAs ternary alloy quantum well optimized for second-order nonlinearity at $10.6 \mu\text{m}$. Starting with a truncated parabolic potential, the final optimized quantum well potential is obtained, with nonlinearity exceeding values previously obtained in the literature.

1. Introduction

Intersubband transitions in semiconductor quantum wells (QW) have attracted considerable research attention. This is mainly due to the large values of the dipole transition matrix elements and the possibility of achieving resonance conditions. Thus, the linear and—to an even greater extent—the nonlinear optical processes in these structures are very intense. Large dipole matrix elements are associated with a small effective mass m^* of electrons, scaling approximately as $m^{*-1/2}$ (reference [1]). Within a given material (i.e., for a given value of m^*), however, a lot can be done to enhance those matrix elements that are relevant to a particular type of nonlinearity, by appropriate shaping of the QW (i.e., its potential), and hence the quantized states' wave functions. While varying the QW shape it is (almost always) essential to keep the level spacing as specified, e.g. equispaced for double-resonant second-harmonic generation (SHG). Clearly, only asymmetric structures are useful for SHG, and these may be realized either by an asymmetric composition grading carried out in a stepwise-constant or continuous manner (see, e.g., references [1] and [2]), or by electric field biasing (see, e.g., reference [3]), or both.

Some considerations regarding optimizing the QW shape, within the class of simple step-graded QWs, and within a somewhat idealized model, were presented in reference [1]. If the

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search for the best potential shape requires any amount of trial-and-error-type calculation, most of the effort is spent in restoring the level spacing upon changing the potential shape, rather than in checking the values of the matrix elements. Within the class of continuously graded QWs, this problem may be very serious. For these we have recently used [4] a method based on supersymmetric quantum mechanics. It starts with a (rather arbitrary) initial potential, such that its quantized states are positioned as required, e.g. are equispaced if the QW is intended for resonance SHG, and then generates a family of potentials isospectral to the initial one, their shape being controlled by one or more scalar parameters. By varying these parameters one may easily search for the potential shape which maximizes those matrix elements relevant for e.g. resonance SHG. Here we describe another method for finding the best potential shape of QWs, which is even more versatile than the one based on supersymmetry. It starts with a completely arbitrary initial potential, and, using the inverse spectral theory (IST) (see, e.g., reference [5]), shifts the states to their desired positions, while, at the same time, it introduces a free parameter (of free parameters) for varying the shape of this modified potential in an isospectral manner. The use of the method is exemplified by using it to find the QW shape for optimal second-order susceptibility, relevant for SHG.

2. The IST tailoring of the potential

The electron motion in a potential well $U(z)$, with a constant effective mass m^* , is described by the envelope function Schrödinger equation

$$-\frac{\hbar^2}{2m^*} \frac{d^2 \psi_i(z)}{dz^2} + U(z) \psi_i(z) = E_i \psi_i(z). \quad (1)$$

The discrete eigenenergies of the system, and the corresponding eigenfunctions, are denoted as E_i and $\psi_i(z)$ ($i = 1, 2, \dots$), respectively. The IST enables one to construct a modified potential $U_{IST}(z)$, which has the property that one (say, the k th) of its eigenvalues is shifted by a prescribed amount ϵ from the k th eigenvalue (E_k) of the initial potential $U(z)$, while all of the other eigenvalues of $U(z)$ and $U_{IST}(z)$ coincide. It has the form

$$U_{IST}(z; E_k + \epsilon) = U(z) - \frac{\hbar^2}{m^*} \frac{d^2}{dz^2} \ln[\mathcal{W}_k\{\psi_\epsilon, \psi_k\}] \quad (2)$$

where $\mathcal{W}_k(z)$ is the Wronskian

$$\mathcal{W}_k\{\psi_\epsilon, \psi_k\} = \psi_\epsilon(z) \frac{d\psi_k(z)}{dz} - \psi_k(z) \frac{d\psi_\epsilon(z)}{dz} \quad (3)$$

with ψ_k being the k th eigenfunction of the initial potential, and ψ_ϵ any solution of the Schrödinger equation with $U(z)$ corresponding to the energy $E_k + \epsilon$. The shift ϵ may take any value in the interval $(E_{k-1} - E_k, E_{k+1} - E_k)$, i.e., the shifted level cannot cross any other level [6].

The function ψ_ϵ , which is clearly not a normalizable eigenfunction, may be written as a linear combination of the two particular solutions, i.e., $\psi_\epsilon = C_1 \varphi_1(z) + C_2 \varphi_2(z)$, satisfying the fundamental initial conditions $\varphi_1(0) = \varphi_2'(0) = 1$ and $\varphi_2(0) = \varphi_1'(0) = 0$.

Consider a system having non-equispaced states, and hence not appropriate for resonant SHG. Its energy spectrum may be ‘corrected’ to provide equal (and just right) spacing between, say, the ground (1) and some other two states (2 and 3) by effecting shifts (one at a time): $E_2 \rightarrow E_2^{\text{shift}} = E_1 + \Delta E$ and $E_3 \rightarrow E_3^{\text{shift}} = E_1 + 2 \Delta E$, where $\Delta E = \hbar \omega$ is the photon energy of the input laser radiation. The values of the shifts of the initial potential states in the above equations are thus $\epsilon_2 = E_2^{\text{shift}} - E_2$ and $\epsilon_3 = E_3^{\text{shift}} - E_3$.

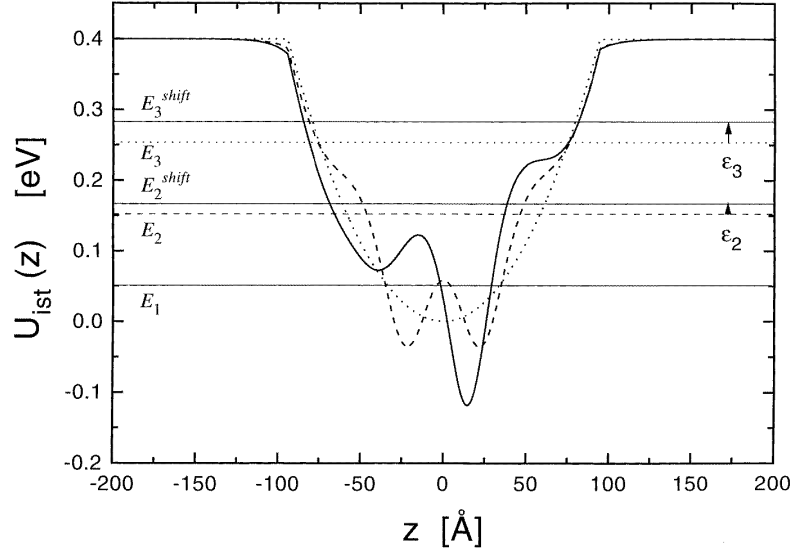


Figure 1. The procedure of level shifting and the potential asymmetrization, causing levels 2 and 3 to shift with respect to the fixed level 1.

If the initial potential is symmetric, and lacks second-order nonlinearity, one also has to build in the asymmetrization in this procedure. For this purpose, the transformation described above is carried out in two steps. First, the wave function ψ_ϵ corresponding to the energy $E_3 + \epsilon_3 = E_1 + 2\Delta E$ is chosen, via the constants $C_1 = 0$ and $C_2 = 1$, to have opposite parity to that of ψ_3 , i.e., to be odd, which delivers a new potential

$$\tilde{U}(z; E_3 + \epsilon_3) = U(z) - \frac{\hbar^2}{m^*} \frac{d^2}{dz^2} \ln[\mathcal{W}_3\{\psi_{\epsilon_3}, \psi_3\}] \quad (4)$$

which, however, is still symmetric, as displayed in figure 1, but has the third state correctly spaced with respect to the ground state: $E_3^{\text{shift}} - E_1 = 2\Delta E$. The normalized wave functions for $i \neq 3$, corresponding to it, are given by

$$\tilde{\psi}_i(z) = \left(1 - \frac{\epsilon_3}{E_i - E_3}\right)^{-1/2} \left[\psi_i(z) - \frac{2m^*\epsilon_3}{\hbar^2} \frac{\psi_{\epsilon_3}(z)}{\mathcal{W}_3\{\psi_{\epsilon_3}, \psi_3\}} \int_{-\infty}^z \psi_i \psi_3 dz' \right] \quad (5)$$

while the wave function for $i = 3$

$$\tilde{\psi}_3(z) = \frac{\psi_3(z)}{\mathcal{W}_3\{\psi_{\epsilon_3}, \psi_3\}} \quad (6)$$

remains to be normalized numerically.

Next comes the asymmetrization. In calculating ψ_{ϵ_2} at the energy $E_2 + \epsilon_2 = E_1 + \Delta E$, the constants $C_{1,2}$ are chosen such that, along with the particular solution having the opposite parity to ψ_2 , the other one having the same parity as ψ_2 (i.e., odd) is also introduced. Indeed, setting $C_1 = 1$ and $C_2 = \alpha$ gives the final potential

$$U_{IST}(z; \alpha, E_3 + \epsilon_3, E_2 + \epsilon_2) = \tilde{U}(z) - \frac{\hbar^2}{m^*} \frac{d^2}{dz^2} \ln[\tilde{\mathcal{W}}_2\{\psi_{\epsilon_2}(\alpha), \tilde{\psi}_2\}] \quad (7)$$

or, after substituting (4) into (7),

$$U_{IST}(z; \alpha) = U(z) - \frac{\hbar^2}{m^*} \frac{d^2}{dz^2} \ln[\mathcal{W}_3\{\psi_{\epsilon_3}, \psi_3\} \tilde{\mathcal{W}}_2\{\psi_{\epsilon_2}(\alpha), \tilde{\psi}_2\}] \quad (8)$$

which is asymmetric for all $\alpha \neq 0$. The corresponding normalized wave functions for $i \neq 2$ read

$$\psi_i^{IST}(z; \alpha) = \left(1 - \frac{\epsilon_2}{E_i - E_2}\right)^{-1/2} \left[\tilde{\psi}_i(z) - \frac{2m^*\epsilon_2}{\hbar^2} \frac{\psi_{\epsilon_2}(z; \alpha)}{\tilde{\mathcal{W}}_2\{\psi_{\epsilon_2}(\alpha), \tilde{\psi}_2\}} \int_{-\infty}^z \tilde{\psi}_i \tilde{\psi}_2 dz' \right] \quad (9)$$

where now $E_3 \equiv E_3^{\text{shift}}$, while the wave function for $i = 2$

$$\psi_2^{IST}(z; \alpha) = \frac{\tilde{\psi}_2(z)}{\tilde{\mathcal{W}}_2\{\psi_{\epsilon_2}(\alpha), \tilde{\psi}_2\}} \quad (10)$$

also remains to be normalized numerically. Equations (8)–(10) are the ‘design’ equations for the final asymmetric potential and the wave functions which enable a finite value of the cyclic product of the matrix elements, relevant for second-order nonlinearity, to be obtained. The free parameter α appearing in (8)–(10) implies the existence of a family of isospectral potentials. By varying α , one also varies the potential shape and hence the wave functions and the dipole matrix elements, with the final aim of finding the optimal $\alpha = \alpha_{opt}$, i.e., the optimized potential $U_{IST}(z; \alpha_{opt})$ which gives the largest product of relevant matrix elements (and resonant second-order nonlinearity). Throughout this variation of α in (8), the energies of its states, and hence the resonance conditions, remain preserved, i.e., $E_2^{\text{shift}} - E_1 = \Delta E$ and $E_3^{\text{shift}} - E_1 = 2\Delta E$.

3. Mapping the variable mass into a constant-mass Hamiltonian

In semiconductor quantum well structures based upon graded semiconductor alloys, it is not only the potential, but also the electron effective mass, that is position dependent. The results of section 2, relying on the constant-mass assumption, are thus likely not to be directly applicable to almost all common QWs (the exception are some specially designed QWs based upon quaternary alloys, for which the effective mass can be kept constant while the potential varies). In technologically more convenient, ternary-alloy-based QWs, the effective mass is necessarily position dependent, as discussed below, and some additional consideration is necessary before one can use the results of section 2 for these structures. The approach that we use is to map the variable-mass Hamiltonian onto one with constant mass. Here we extend the consideration presented in reference [8] to include the cases of truncated and asymmetric potentials.

Consider a QW based upon a ternary semiconductor alloy $A_xB_{1-x}C$, with the mole fraction varying along the z -axis, i.e., $x = x(z)$. We take the conduction band edge in the BC compound to be lower by ΔV than that in the AC compound, while the electron effective masses in the two are m_{BC} and m_{AC} , respectively. Then the potential experienced by the electrons (the conduction band edge), and their effective mass both vary along the z -axis as $V(z) = \Delta V x(z)$, and $m(z) = m_{AC}x(z) + m_{BC}[1 - x(z)]$. Thus, in ternary alloys the potential and the effective mass are related as

$$V(z) = (\Delta V/\Delta m)[m(z) - m_{BC}] = \theta[m(z) - m_{BC}]$$

where $\Delta m = m_{AC} - m_{BC}$ and $\theta = \Delta V/\Delta m$.

With the position-dependent effective mass, the Schrödinger equation for the envelope functions has the Ben Daniel–Duke form [7], i.e., with the notation introduced above:

$$\frac{d}{dz} \left(\frac{1}{m(z)} \frac{d\psi(z)}{dz} \right) + a[E - \theta(m(z) - m_{BC})]\psi(z) = 0 \quad (11)$$

where $a = 2m_0/\hbar^2$, and m_0 is the free-electron mass. Now we aim at finding the function $m(z)$, and, uniquely related to it, $V(z)$ and $x(z)$, such that the eigenstates of equation (11) are identical to those of the constant-mass equation (8) with the potential $U_{IST}(z)$ specified in advance. For this purpose we introduce a new coordinate y , such that $z = f(y)$, where the function $f(\cdot)$ will be specified later. In terms of this new coordinate, equation (11) takes the form

$$\frac{d^2 u(y)}{dy^2} + \{A(y) + am(y)f'^2(y)[E - \theta(\underline{m}(y) - m_{BC})]\} u(y) = 0 \quad (12)$$

with

$$A(y) = -\frac{1}{4} \left(\frac{d \ln[\underline{m}(y)f'(y)]}{dy} \right)^2 + \frac{1}{2} \frac{d^2 \ln[\underline{m}(y)f'(y)]}{dy^2} \quad (13)$$

where

$$u(y) = \text{constant} \times \underline{\psi}(y) / \sqrt{\underline{m}(y)f'(y)}$$

and

$$\begin{aligned} \underline{\psi}(y) &= \psi[f(y)] = \psi(z) \\ \underline{m}(y) &= m[f(y)] = m(z) \\ f'(y) &= df(y)/dy. \end{aligned}$$

Equations (11) and (12) clearly have identical spectra.

Now we require the constant-mass ($m^* = m_{BC}$) Schrödinger equation with the optimized potential $U_{IST}(y, \alpha_{opt})$, equation (8), to coincide with equation (12). This results in a system of two equations, from which we find

$$\underline{m}(y) = \frac{1}{4am_{BC}\theta} v^{-2}(y) \quad (14)$$

$$z = f(y) = \int_0^y \sqrt{\frac{m_{BC}}{\underline{m}(y')}} dy'. \quad (15)$$

where the function $v(y)$ in equation (14) is found by solving the nonlinear differential equation

$$2v(y) \frac{d^2 v(y)}{dy^2} - \left(\frac{dv(y)}{dy} \right)^2 - 4am_{BC}[\theta m_{BC} + V(y)]v^2(y) + 1 = 0. \quad (16)$$

Equation (16) may be solved by first finding the particular solutions $\zeta_{L,R}(y)$ of the characteristic equation [9] (here we specialize to the case of a truncated potential $V(y) = V = \text{constant}$ for $|y| > \Delta$, and $V(y) = U_{IST}(y, \alpha_{opt})$ for $|y| < \Delta$):

$$\begin{aligned} \frac{d^2 \zeta(y)}{dy^2} - am_{BC}[\theta m_{BC} + V]\zeta(y) &= 0 & |y| > \Delta \\ \frac{d^2 \zeta(y)}{dy^2} - am_{BC}[\theta m_{BC} + U_{IST}(y, \alpha_{opt})]\zeta(y) &= 0 & |y| < \Delta \end{aligned} \quad (17)$$

chosen such that their Wronskian squared equals unity. In analogy to scattering theory, the two linearly independent solutions of equation (17) may be written as ($\kappa^2 = am_{BC}[\theta m_{BC} + V]$)

$$\zeta_{L,R}(y) = \begin{cases} \exp(\kappa y) + R_L \exp(-\kappa y) & T_R \exp(-\kappa y) & y < -\Delta \\ A_{L,R} s_1(y) + B_{L,R} s_2(y) & & -\Delta < y < \Delta \\ T_L \exp(\kappa y) & R_R \exp(\kappa y) + \exp(-\kappa y) & y > \Delta \end{cases} \quad (18)$$

where $s_{1,2}(y)$ are the particular solutions of (17), satisfying the fundamental initial conditions $s_1(0) = s_2'(0) = 1$ and $s_2(0) = s_1'(0) = 0$, and may be found numerically, while the constants $T_{L,R}$, $R_{L,R}$, $A_{L,R}$ and $B_{L,R}$ are determined from the Wronskian properties and the boundary conditions at $y = \pm\Delta$. These constants depend slightly on the choice of Δ , but this dependence becomes diminishingly weak as Δ increases. We also use the fact that $T_L = T_R = T$.

Since the Wronskian squared of ζ_L and ζ_R equals unity, in terms of the two particular solutions of (17) the general solution of equation (16) may be written as [9]

$$v(y) = [C_e \zeta_L^2(y) \pm \sqrt{1 + 4C_e C_o} \zeta_L(y) \zeta_R(y) + C_o \zeta_R^2(y)] / (2\kappa T) \quad (19)$$

where $C_{e,o}$ are constants to be determined. Now, having in mind the physically acceptable values of the QW parameters, i.e., $m(|y| \rightarrow \infty) = V(\Delta m / \Delta V) + m_{BC} = m_b$ and $V(|y| \rightarrow \infty) = V$, and accounting for the asymptotic behaviour of $\zeta_{L,R}(y)$, we find that the condition $v(|y| \gg \Delta) \rightarrow \text{constant} \neq 0$ is satisfied by the choice of constants

$$C_o = \pm \frac{T R_L}{(R_R R_L - T^2)} \quad C_e = \pm \frac{T R_R}{(R_R R_L - T^2)}. \quad (20)$$

Finally, substitution into equation (14) gives the effective-mass variation

$$\underline{m}(y) = m_b \left/ \left[1 + \frac{R_{R,L}}{(R_R R_L - T^2)} \exp(\pm 2\kappa y) \right]^2 \right. \quad |y| > \Delta \quad (21)$$

where the subscripts R (L) and $+$ ($-$) in the exponential refer to $y < -\Delta$ ($y > \Delta$), and

$$\underline{m}(y) = \frac{m_b T^2 (R_R R_L - T^2)^2}{[T R_R \zeta_L^2(y) - (R_R R_L + T^2) \zeta_L(y) \zeta_R(y) + T R_L \zeta_R^2(y)]^2} \quad |y| < \Delta. \quad (22)$$

The real-space variation of the effective mass, $m(z) = m[f(y)] = \underline{m}(y)$, may then be found from (15) and (21)–(22) numerically, and then the potential $V(z)$ and the grading function $x(z)$ directly follow, e.g.

$$V(z) = V[z(y)] = \underline{V}(y) = \frac{\Delta V}{\Delta m} [\underline{m}(y) - m_{BC}]. \quad (23)$$

The final Hamiltonian has the effective mass following the potential, as is appropriate for ternary-alloy-based QWs, and is fully isospectral with the Hamiltonian with the constant effective mass $m^* = m_{BC}$ and the optimized potential $U_{IST}(y, \alpha_{opt})$ (equation (8)). Its normalized wave functions are given by

$$\underline{\psi}_i(y) = [\underline{m}(y) / m_{BC}]^{1/4} \psi_i^{IST}(y) \quad (24)$$

in parametric form, i.e., with $z = f(y)$ (equation (15)). The wave functions $\psi_i^{IST}(y)$ (equations (9) and (10)) are here assumed to be already normalized, i.e., we assume that $\int |\psi_i^{IST}(y)|^2 dy = 1$.

4. Numerical results and discussion

To illustrate the above consideration, we have performed optimization calculations to design a QW structure for double-resonance SHG of CO₂ laser radiation ($\hbar\omega = \Delta E = 116$ meV). Taking the lowest three levels to be relevant in this process, a well depth of at least 400 meV is necessary to accommodate these levels, and the compounds AC and BC should be chosen accordingly. The commonly used Al_xGa_{1-x}As system meets this requirement, and has the additional advantages that it is strain-free, and technologically well understood, so it was chosen for further work. The conduction band Γ -valley discontinuity is $\Delta V = 750$ meV,

and the electron effective masses of the two compounds are $m_{\text{GaAs}} = 0.066 m_0$ and $m_{\text{AlAs}} = 0.15 m_0$ [7].

In QWs with Γ -valley-related levels, it is only the z -component (perpendicular to the QW layer) of the electric field that is active in intersubband transitions. Considering the process of SHG, the second-order nonlinear susceptibility, that relates the field at the pump frequency and the polarization at the harmonic frequency, is largest under double-resonance conditions, i.e., $E_2 - E_1 = E_3 - E_2 = \hbar\omega$, and then its only relevant component amounts to

$$\chi_{zzz}^{2\omega} = \frac{e^3(\rho_{11} - \rho_{22})}{L_z \epsilon_0} \frac{\mu_{12}\mu_{23}\mu_{31}}{(\hbar\Gamma_2)^2} \quad (25)$$

where $\mu_{ij} = \langle i|z|j \rangle$ are the transition matrix elements (dipole moments), L_z denotes the QW structure width, ρ_{ii} is the electron density in state i per unit well surface, $\hbar\Gamma_2$ is the linewidth (taken as common to all transitions). By varying the QW profile (potential shape) one varies the dipole moments, while the linewidth is affected far less significantly. Therefore, maximizing $\chi_{zzz}^{2\omega}$ effectively amounts to maximizing the cyclic product of matrix elements, $\Pi^{(2)} = \mu_{12}\mu_{23}\mu_{31}$, in the numerator of (25).

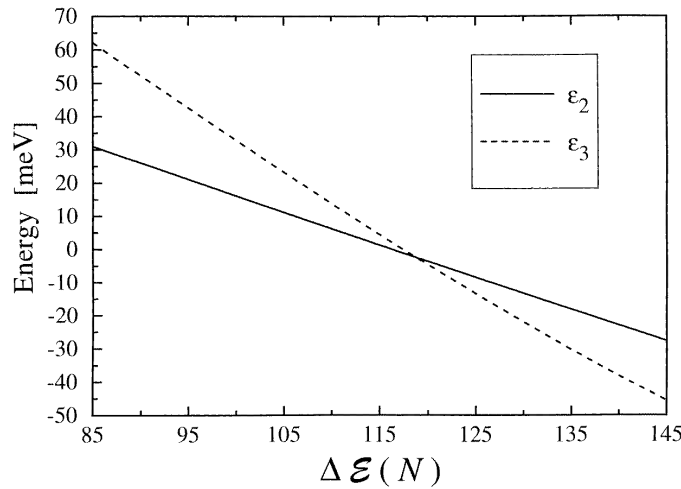


Figure 2. The dependences of the shifts $\epsilon_2 = E_2^{\text{shift}} - E_2$ and $\epsilon_3 = E_3^{\text{shift}} - E_3$, of levels 2 and 3, necessary to obtain equal spacings (double resonance), on the parabolic potential slope $\Delta\mathcal{E}$.

To find the optimized asymmetric potential, with the largest $\Pi^{(2)}$, we start from a family of truncated parabolic potentials of the form

$$U(z) = \begin{cases} \frac{m^*}{2} \left(\frac{\Delta\mathcal{E}(N)}{\hbar} \right)^2 z^2 & |z| < \Delta \\ V & |z| > \Delta \end{cases} \quad (26)$$

where $\Delta\mathcal{E}(N) = 84.75 + 0.25N$ (meV), and N is an integer incremented from 1 to 241. The effective mass in (26) is taken as constant and equal to that in GaAs, and the potential is truncated at $V = 400$ meV (hence the well width Δ changes with incrementing N). Because of truncation this is not exactly a linear harmonic oscillator, and in no case will the levels be strictly equispaced. Furthermore, their energies will change as N (i.e., the well width) varies, so none of the potentials (26) meets the double-resonance condition. Applying

an isospectral transform like supersymmetry [10] will make them asymmetric, and all μ_{ij} would then be nonzero, but will not correct the level's energies. The dependences on the frequency $\Delta\mathcal{E}/\hbar$ of the deviations of these energies from their desired positions that would provide double resonance at $\hbar\omega = 116$ meV (i.e., in the spirit of section 2, the necessary shifts $\epsilon_2 = E_2^{\text{shift}} - E_2$ and $\epsilon_3 = E_3^{\text{shift}} - E_3$) are given in figure 2.

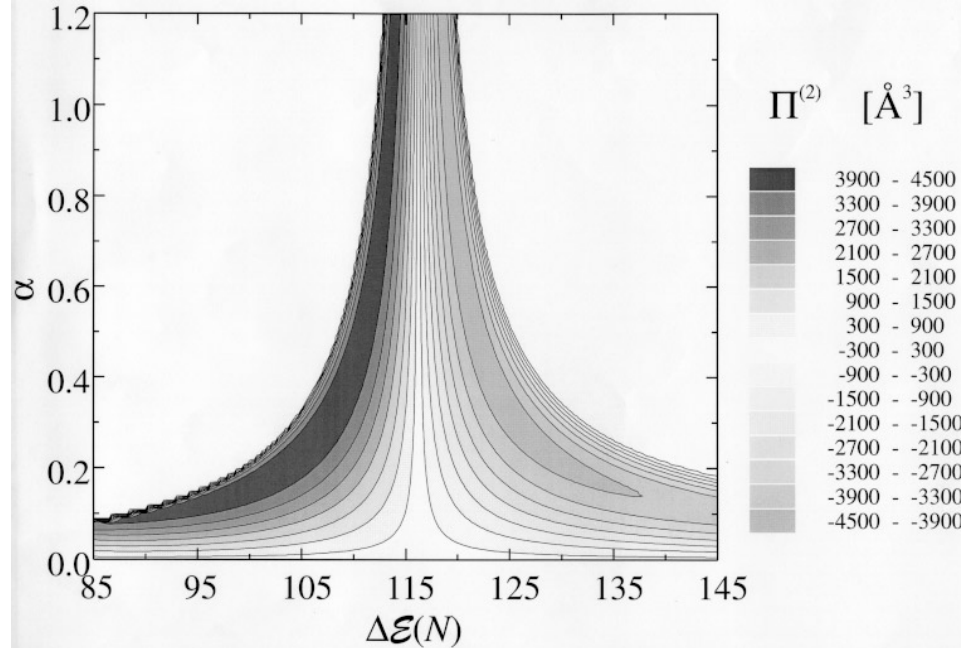


Figure 3. Values of the matrix element product $\Pi^{(2)} = \mu_{12}\mu_{23}\mu_{31}$ obtainable with various values of the QW design parameters $\Delta\mathcal{E}(N)$ and α .

The initial potentials are then processed along the lines presented in section 2: the third level of $U(z)$ is shifted such that it is separated by 232 meV from the first, i.e., $E_3^{\text{shift}} = E_3 + \epsilon_3 = E_1 + 232$ meV, and, by adjusting the constants, the parity of its wave function is set opposite to that of $\psi_3(z)$. Next, the second level is shifted according to $E_2^{\text{shift}} = E_2 + \epsilon_2 = E_1 + 116$ meV. This procedure was repeated for all potentials in the family (26), and in each case the asymmetrization parameter α was varied while monitoring the value of the matrix element product $\Pi^{(2)}$ (calculated by using equations (9) and (10)). With the initial potentials chosen symmetric, it is enough to give only positive values to the parameter α , because here $\Pi^{(2)}(-\alpha) = -\Pi^{(2)}(\alpha)$; otherwise both positive and negative values should be explored. We should also note here that, in doing these calculations, one has to be careful that the Wronskians in equations (4)–(10) do not cross zero, in order to avoid singularities and physically unacceptable solutions. The results of this search are displayed in figure 3. The largest value of $\Pi^{(2)}$ is found with the parameter values $N = 68$ (i.e., $\Delta\mathcal{E}(68) = 101.75$ meV) and $\alpha_{opt} = 0.18$. Here we have $\Pi^{(2)} = 4375.2 \text{ \AA}^3$, with individual dipole moments $\mu_{12} = 16.96 \text{ \AA}$, $\mu_{23} = 28.12 \text{ \AA}$ and $\mu_{31} = 9.17 \text{ \AA}$. The corresponding optimized potential $U_{IST}(z; \alpha_{opt})$ is given in figure 4. It may be of interest to note that the original potential, from which this optimized potential was derived, had its levels at $E_1 = 50.87$ meV, $E_2 = 152.54$ meV and $E_3 = 253.45$ meV; therefore (with $\Delta E_{21} = 101.67$ meV and $\Delta E_{32} = 100.91$ meV) it was not matched for resonant SHG

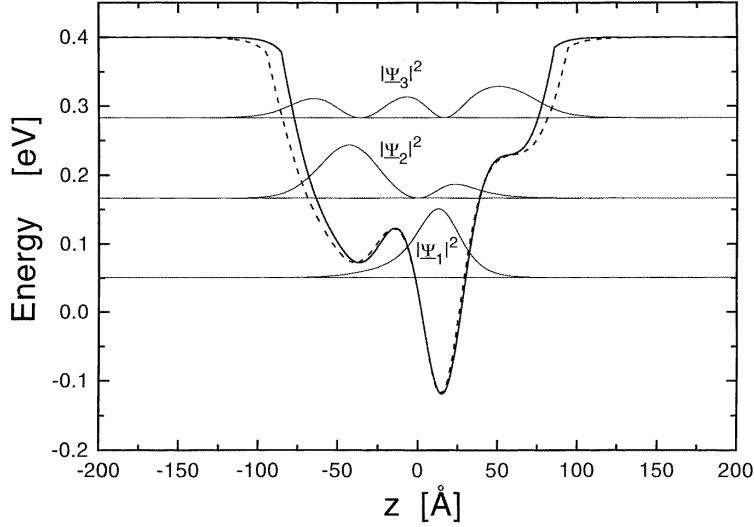


Figure 4. The optimized potential $U_{IST}(z)$, corresponding to $\Delta\mathcal{E} = 101.75$ meV and $\alpha_{opt} = 0.18$, with constant effective mass, and the optimized realizable potential $V(z)$ with the variable effective mass following it, as is appropriate for a graded AlGaAs alloy.

of $\hbar\omega = 116$ meV radiation, and its asymmetrization via the isospectral supersymmetric transform alone would not help. However, the IST-based level shifts, accompanied by asymmetrization, produced the desired outcome.

The potential optimized so far, assuming a constant effective mass, is not directly realizable in graded ternary alloys, because the effective mass there cannot be kept constant. To make it realizable, we have to map the Hamiltonian with $U_{IST}(z; \alpha_{opt})$ and $m^* = \text{constant}$ into the Hamiltonian with the effective mass following the potential, as is appropriate for the chosen ternary alloy system. This mapping is carried out along the lines described in section 3, in particular by equations (21)–(23) and (15). The optimized Hamiltonian realizable in graded $\text{Al}_x\text{Ga}_{1-x}\text{As}$ having been obtained, it remains to check the product of the matrix elements for this new (but realistic) system. Using equation (24) we find that the matrix elements

$$\mu_{ij} = \langle \underline{\psi}_i(y) | z(y) | \underline{\psi}_j(y) \rangle$$

now amount to $\mu_{12} = 16.31 \text{ \AA}$, $\mu_{23} = 25.86 \text{ \AA}$ and $\mu_{31} = 9.27 \text{ \AA}$, so $\Pi^{(2)} = 3910 \text{ \AA}^3$ has somewhat decreased from what was predicted above. This should have been expected, since the effective mass throughout the structure generally exceeds the constant value $m^* = 0.066$ initially taken, and $\mu \sim m^{-1/2}$ (reference [1]). The realistic optimized potential, given in figure 4, has a negative undershoot, and hence has a somewhat larger span of values than the original $U(z)$. However, the negative undershoot itself makes no difficulties in the realization, because the reference zero of the potential is irrelevant for the physics, and the whole picture may be shifted up or down at will. In realizing this potential by grading the $\text{Al}_x\text{Ga}_{1-x}\text{As}$ alloy, via the relation $x(z) \Delta V = V(z) + \text{constant}$, one may set constant = $|\min(V(z))|$, so that $x = 0$ at the lowest point of the well, and the full potential span offered by $\text{Al}_x\text{Ga}_{1-x}\text{As}$ is taken advantage of.

Comparison of the maximal value of $\Pi^{(2)}$ found here against the best values obtained elsewhere for step-graded QWs (e.g. $\Pi^{(2)} = 2394 \text{ \AA}^3$, in reference [1], or $\Pi^{(2)} = 2635 \text{ \AA}^3$,

in reference [11]) shows that $\Pi^{(2)}$ obtained in this work (though in a continuously graded QW) is better by $\sim 30\%$. We should also note that, in the case of deeper wells, one would have to account for the bulk nonparabolicity. It cannot be directly included in the theory described above because an energy-dependent potential would result, and this effect would be better accounted for by slight numerical ‘repolishing’ of the optimized potential obtained without it. Our previous experience with SUSYQM-based QW optimization as regards second-harmonic generation [4] indicates that such ‘repolishing’ has a rather mild influence on the best potential shape (slightly squeezing the output of idealized calculations in order to compensate for the nonparabolicity-increased effective mass).

It should be noted that the particular schedule of steps used above is just one among several possibilities. To achieve the required positions of the three levels, one may choose to fix the second or the third, and shift the other two, which would produce a potential different from the one obtained here. Furthermore, additional freedom may be gained by introducing more free constants when constructing the ψ_ϵ -functions from the fundamental solutions. This should be done with great care, however, because e.g. introducing a parameter β in ψ_{ϵ_3} (analogous to α in ψ_{ϵ_2}) would result in a highly oscillatory term $(d^2/dz^2) \ln[W\{\psi_3, \psi_{\epsilon_3}\}]$, which would eventually yield a highly oscillatory, and difficult to realize, final potential.

5. Conclusion

A procedure for the design of quantum well structures optimized as regards intersubband double-resonant second-harmonic generation was proposed and discussed. Starting with an arbitrary potential, with level energies not properly positioned for this application, this procedure allows one to shift the relevant levels to the desired positions, by using the inverse spectral theory, and vary the potential shape, controlled by free parameters, in order to find the shape that maximizes the matrix elements relevant for second-harmonic generation. Furthermore, the procedure is devised to handle the case of position-dependent effective mass, and is thus applicable to realistic QW structures. Its applicability was demonstrated by designing a graded AlGaAs ternary alloy quantum well optimized as regards second-order nonlinearity at $10.6 \mu\text{m}$. Starting with a truncated parabolic potential, the final optimized QW potential that was obtained had a second-order susceptibility significantly ($\sim 30\%$) exceeding values previously obtained in the literature, and is slightly better than that obtained in reference [4].

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