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Multiparameter optimization of optical nonlinearities in semiconductor quantum wells by supersymmetric quantum mechanics

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Abstract

The multiparameter procedure of semiconductor quantum well profile optimization, using the supersymmetric quantum mechanics, is described and explored. The method generates families of isospectral potentials that depend on a specified number of scalar parameters, which are then varied so to maximize the desired property of the system, in this case the nonlinear susceptibility $\chi_0^{(2)}$ which gives rise to the optical rectification. The merits and limits of the multiparameter procedure are discussed. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

Intersubband optical transitions in quantum well (QW) structures are continuously attracting the research attention in the last two decades. Due to considerable values of dipole transition matrix elements the QWs have quite remarkable linear and nonlinear optical properties. Various effects in QWs may be enhanced by suitably tailoring their electronic structure ("band structure engineering"). A particular effect may be grossly enhanced by achieving the resonance conditions, i.e., appropriate spacings between the most relevant states, and also by tailoring the wave functions so that the (combinations of) matrix elements relevant for this particular effect are maximized [1]. This is particularly important for higher order nonlinear processes. Optimization of simple stepwise-constant profiled QWs has been considered quite some time ago [2], while the optimization of continuously graded structures required more sophisticated techniques like the supersymmetric quantum mechanics (SUSYQM) and the inverse spectral theory (IST), e.g., Ref. [3]. Previously, however, these methods have been employed only for single-parameter optimization, i.e., the QW profile was controlled via a single scalar parameter. In this Letter we develop a multiparameter procedure, and apply it to the problem of optimizing the QW profile so to maximize the optical rectification co-

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efficient. Our aim is to explore to what extent the increased versatility of the potential tailoring leads to an improvement of the final optimized design of the potential.

2. Theoretical considerations

An electric field $E(t) = E_0 \cos(\omega t)$ incident on the QW induces the polarization response:

$$P(t) = \epsilon_0\big(\chi_\omega^{(1)} E_0 \exp(j\omega t) + \chi_{2\omega}^{(2)} E_0^2 \exp(2j\omega t) + \chi_0^{(2)} E_0^{(2)}\big) + \text{c.c.}, \tag{1}$$

where ϵ_0 is the dielectric susceptibility of vacuum and $\chi_\omega^{(i)}$ is the ith order susceptibility at frequency ω. Considering the n-doped semiconductor QWs, and the incident photon energies well below the band gap, the polarization response is predominantly determined by intersubband transitions, between the quantized states within the conduction band. The optical rectification is described by the $\chi_0^{(2)}$ term, which, under the resonance conditions ($\hbar\omega = E_2 - E_1$, where $E_{1,2}$ are energies of the two quantized states involved) reads [2]

$$\chi_0^{(2)} = \frac{e^3 T_1 T_2}{2\epsilon_0 \hbar^2}(N_1 - N_2)\mu_{12}^2 \delta_{12}, \tag{2}$$

where $\delta_{12} = \langle 1|z|1\rangle - \langle 2|z|2\rangle$ is the (difference of) permanent dipole moments, $\mu_{12} = \langle 1|z|2\rangle$ the transition dipole moment, N_1 and N_2 the electron densities in states 1 and 2 per unit well surface, while T_1 and T_2 denote the diagonal and off-diagonal relaxation times in the Liouville equation (describing the state lifetime and the transition linewidth, respectively). The quantities $N_1 - N_2$, T_2, and to some extent T_1 are not too sensitive to the QW profile, and the maximization of $\chi_0^{(2)}$ essentially reduces to the maximization of the product $\Pi = \mu_{12}^2 \delta_{12}$.

For the initial potential we here choose the Pöschl–Teller potential, since much of the work can then be done analytically. It reads

$$U(z) = -\frac{U_0}{\cosh^2(\alpha z)}, \tag{3}$$

the bound states of which are known analytically [4]:

$$E_i = -\frac{\alpha^2}{\beta}(S - i)^2, \quad i = 0, 1, 2, \ldots, \tag{4}$$

where

$$S = \frac{\sqrt{1 + 4U_0\beta/\alpha^2} - 1}{2} \tag{5}$$

and $\beta = 2m^*/\hbar^2$. The parameter S determines the number of bound states N_B, supported by this potential:

$$N_B = \begin{cases} 1 + \text{Int}[S], & S \notin \mathcal{N}, \\ S, & S \in \mathcal{N}, \end{cases} \tag{6}$$

where $\mathcal{N} = \{1, 2, 3, \ldots\}$. The eigenfunctions for these states are also known analytically [4], though the corresponding expressions will not be reproduced here. By choosing appropriate values of the parameters α and U_0 one can tailor the potential to support exactly the required number of bound states, and set the spacing between two specified states.

We transform this potential according to the expressions given, e.g., in Refs. [3] and [5]. By deleting and restoring a bound state at energy E_k, with the eigenfunction ψ_k, via SUSYQM, we derive a single-parameter family of isospectral potentials $U_{SS}(\lambda_k, z)$ [5]:

$$U_{SS}(\lambda_k, z) = U(z) - \frac{\hbar^2}{m^*}\frac{d^2}{dz^2}\ln\left[\lambda_k + \int_{-\infty}^{z} \psi_k^2\, dz\right], \quad \lambda_k \notin (-1, 0). \tag{7}$$

Noteworthy, for symmetric $U(z)$ it suffices to vary λ_k over positive values only, since the situation is just spatially reversed for negative values. The solution to the Schrödinger equation with a constant effective mass m^* and the potential $U_{SS}(\lambda_k, z)$,

$$\frac{d^2\psi_i}{dz^2} + \frac{2m^*}{\hbar^2}\big[E_i - U_{SS}(\lambda_k, z)\big]\psi_i(z) = 0, \tag{8}$$

is the set of normalized wave functions given by

$$\psi_{iSS}(\lambda_k, z) = \psi_i(z) - \frac{\psi_k(z)}{\lambda_k + \int_{-\infty}^{z} \psi_k^2\, dz} \times \int_{-\infty}^{z} \psi_i(z)\psi_k(z)\, dz, \quad i \neq k, \tag{9}$$

$$\psi_{kSS}(\lambda_k, z) = \sqrt{\lambda_k(\lambda_k + 1)}\,\frac{\psi_k(z)}{\lambda_k + \int_{-\infty}^{z} \psi_k^2\, dz}, \quad i = k. \tag{10}$$

Iterative application of the above expressions will bring in more free parameters, one at a time. In effect,

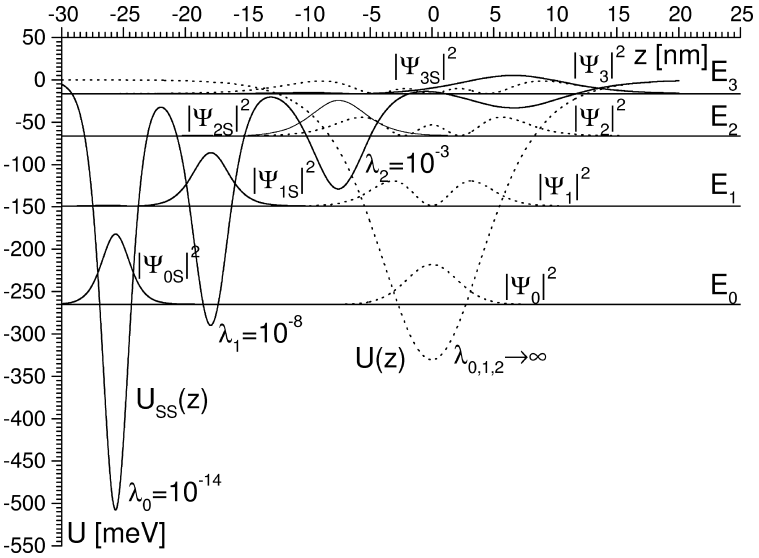

Fig. 1. The initial Pöschl–Teller potential $U(z)$ with four bound states and the corresponding wave functions ψ_i squared (dashed lines), and the isospectrally transformed potential $U_{SS}(z)$ with the corresponding wave functions ψ_{iSS}, obtained with values of the transform parameters given in the figure (solid lines).

using U_{SS} and one of $\psi_{iSS}(\lambda_k, z)$ instead of $U(z)$ and $\psi_k(z)$ in Eq. (7), which corresponds to deleting and restoring a state at E_i of the potential $U_{SS}(\lambda_k, z)$, we derive the two-parameter family $U_{SS}(\lambda_k, \lambda_i, z)$, etc. All these potentials are isospectral.

3. Numerical results and discussion

Numerical calculations were performed starting with GaAs based QWs ($m^* = 0.067$) with 2, 3, or 4 bound states, with parameters α and U_0 chosen, via Eqs. (4)–(6), so that the levels spacing $\Delta E_{10} = 116$ meV (the CO_2 laser radiation). Thus, for the 2-level QW we have set $\alpha = 0.264$ nm^{-1} and $U_0 = 232$ meV, obtaining $E_0 = -154.7$ meV and $E_1 = -38.7$ meV; for the 3-level QW, $\alpha = 0.206$ nm^{-1} and $U_0 = 278.4$ meV, with $E_0 = -208.8$ meV, $E_1 = -92.8$ meV, and $E_2 = -23.2$ meV; for the 4-level QW, $\alpha = 0.174$ nm^{-1} and $U_0 = 331.4$ meV, with $E_0 = -265.1$ meV, $E_1 = -149.1$ meV, $E_2 = -66.3$ meV, and $E_3 = -16.6$ meV. Out of these states, if more than two, only the lowest two states (labelled as 0 and 1) are relevant for the process of interest, but any of them may be used as factorization states in course of tailoring the initial potential.

Next we do the SUSYQM transform(s), as described in the preceding section, and find the potentials $U_{SS}(\lambda_i, z)$, where $i \in \{0, 1\}$, for the 2-level QW, $U_{SS}(\lambda_i, \lambda_j, z)$, where $i, j \in \{0, 1, 2\}$, $i \neq j$, for the 3-level QW, and $U_{SS}(\lambda_i, \lambda_j, \lambda_k, z)$, where $i, j, k \in \{0, 1, 2, 3\}$, $i \neq j \neq k$, for the 4-level QW, as well the corresponding wave functions, Eqs. (9) and (10).

The influence of the parameter λ_k on the potential shape may be analysed from Fig. 1. Here we have a 4-level QW, with $\Delta E_{10} = 116$ meV, in its original form and as transformed by deleting and restoring states at E_k, $k = 0, 1, 2$. The parameters λ_k appearing in this process start influencing the potential profile only when they become small (i.e., the potential is simply reproduced in the limit $\lambda \to +\infty$). As a particular $\lambda_k \to 0$, however, the potential becomes considerably distorted from the original one (the same applies to the limit $\lambda_k \to -1$, if λ_k is taken to be negative. This happens in such a way that it is the state at E_k which is mostly affected, its wave function becoming increasingly confined to the local "pit" of the potential, emerging, moving away, and becoming deeper when λ_k decreases. At the limiting value

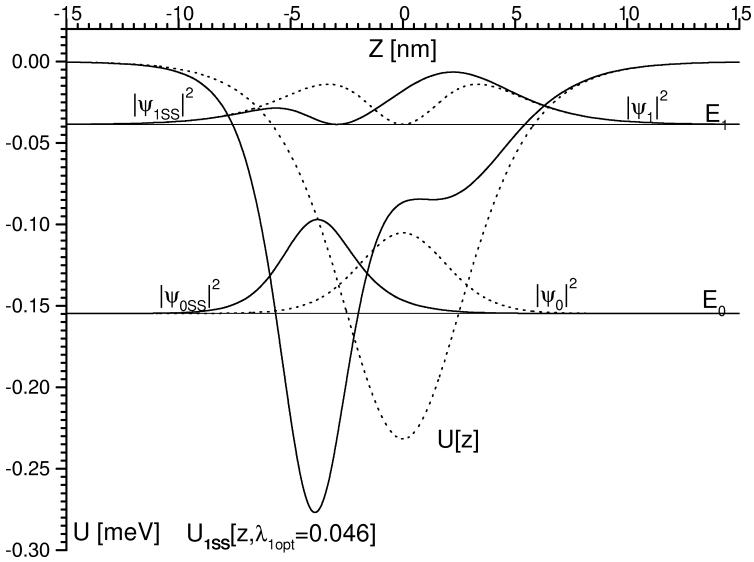

Fig. 2. The initial Pöschl–Teller potential with two bound states and wave functions (dashed), and the corresponding SUSYQM partner quantities (solid lines), obtained for the parameter λ_0 which maximizes the value of $\Pi = \mu_{12}^2 \delta_{12}$.

$\lambda_k = 0$ the shift of this wave function becomes infinite, which is equivalent to complete deletion of this state. Therefore, among the permanent dipole moments, λ_k has a drastic influence on $\langle k|z|k\rangle$, though it also affects somewhat the other ("nonparametrized") states, which experience a limited shift in the opposite direction, and decreasing their amplitudes in the region where ψ_{kSS} peaks. Consequently, the differences $\langle k|z|k\rangle - \langle \ell|z|\ell\rangle$ will increase, but the transition dipole moments that involve the state k will decrease, because of the decreasing overlap of the corresponding wave functions. The product $\Pi = \mu_{12}^2 \delta_{12}$ will therefore be small for $\lambda_k \to 0$, and it was also small (or zero, for symmetric initial potential) before any deformation was made, so it is clear there must be an optimum for some "intermediate" value of λ_k. When a new parameter is introduced and varied, the way it affects "its own" and "other" states repeats, but the total effect upon the combination of matrix elements may not be quite obvious.

This type of behaviour may be seen from Figs. 1–4. With this in mind, it should be clear that introducing more parameters than is the number of relevant states (provided the QW enables it, by supporting enough states) may not bring in any improvement in the value of Π. Indeed, we find that the optimal potential may be generated with infinitely many combinations of λ_1, λ_2, λ_3, and λ_4, the mutual difference being just that such potentials are translated along the z axis by different amounts, which has no physical significance. Therefore, varying a smaller number of parameters (even if more are available) is practically enough for optimization. However, the choice of which of them are to be varied is not quite trivial — the final results may depend on this choice, as we demonstrate below.

To find the efficiency of the optimization procedures with reduced number of parameters, in Fig. 2 we display the initial 2-level Pöschl–Teller potential and its optimized transformed partner $U_{SS}(\lambda_0, z)$ which maximizes Π (to $\Pi(\lambda_0) = 13.54$ nm^3, for $\lambda_0 = 0.266$). The opposite directions of the wave functions shifts are clearly visible in Fig. 2. The same value of Π was also obtained by varying λ_1 only, not λ_2, the optimal value now being $\lambda_1 = 0.0463$, and the same result also was reproduced in the two-parameter procedure, for $\lambda_0 = 0.48$ and $\lambda_1 = -1.58$. The dependence of the product Π on λ_0 in this system is given in Fig. 5, and that for the individual components, μ_{12} and δ_{12}, in Fig. 6.

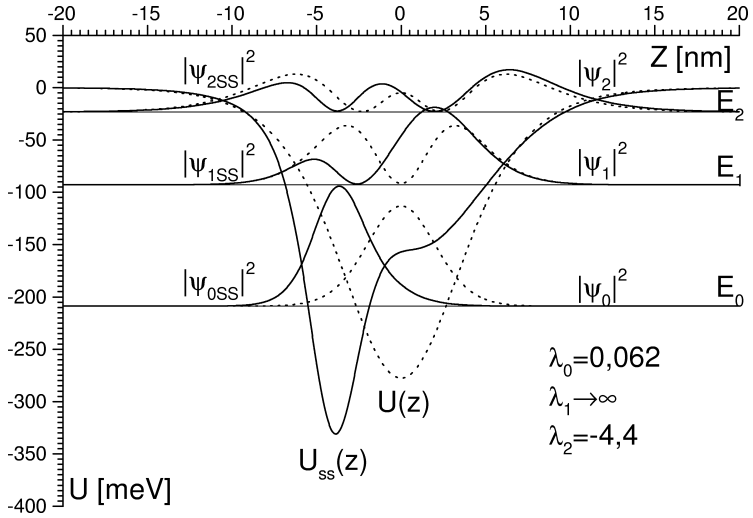

Fig. 3. Same as Fig. 2, but for the potential with three bound states, and two parameters are involved.

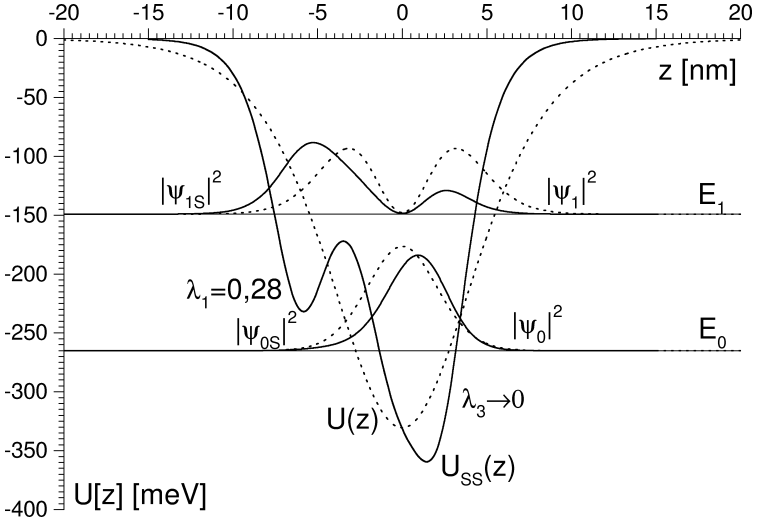

Fig. 4. Same as Fig. 2, but for the potential with four bound states, and two parameters are involved.

In Fig. 3 we give the initial 3-level Pöschl–Teller potential and its optimized transformed partner $U_{SS}(\lambda_0, \lambda_2, z)$ which maximizes Π (for $\lambda_0 = 0.062$ and $\lambda_2 = -4.4$). Here we found that the variation of λ_0 and λ_2 gives the best result ($\Pi = 12.98\,\text{nm}^3$), while varying λ_0 and λ_1, or λ_1 and λ_2 delivered only slightly smaller Π (12.92 and 12.58 nm^3, respectively). On the other hand, varying just a single parameter was less effective, giving $\Pi = 11.17$, 11.64, and 7.42 nm^3 for $\lambda_0 = 0.068$, $\lambda_1 = -1.27$, and $\lambda_2 = 0$, respectively. Therefore, the 2-parameter procedure improves the result of the 1-parameter procedure by (practically significant) ≈10%. By varying all the three parameters, however, no further improvement was made. The dependences $\Pi(\lambda_0)$, $\delta_{12}(\lambda_0)$, and $\mu_{12}(\lambda_0)$, for $\lambda_2 = -4.4$, are given in Figs. 5 and 6.

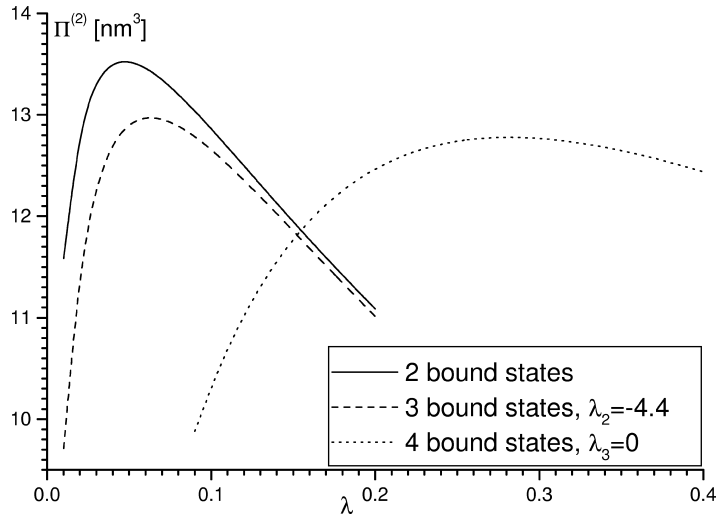

Fig. 5. The dependence of $\Pi = \mu_{12}^2 \delta_{12}$ on the parameter(s) λ used in optimization of wells with two (solid), three (dashed) and four (dotted) bound states.

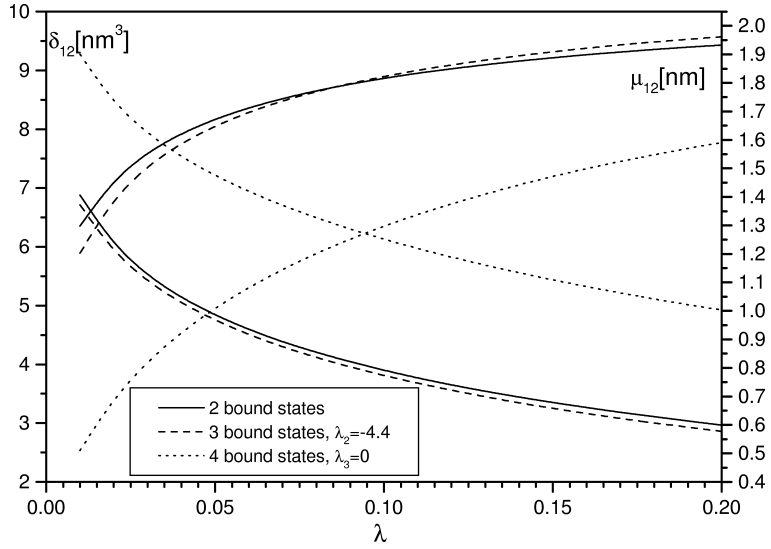

Fig. 6. Same as in Fig. 5, but for the individual matrix elements δ_{12} and μ_{12}.

In Fig. 4 are displayed the initial 4-level Pöschl–Teller potential and its optimized transformed partner $U_{SS}(\lambda_1, \lambda_3, z)$. The best result obtained with the 3-parameter optimization here was $\Pi(\lambda_0 = 1.80, \lambda_1 = -1.28, \lambda_2 = -1.92) = 12.72$ nm^3, but this turned out to be slightly less than what was obtained in the 2-parameter procedure with λ_1 and λ_3, which gave the largest value $\Pi(\lambda_1 = 0.28, \lambda_3 = 0) = 12.78$ nm^3. This implies that the optimized potential in fact supports three bound states, the fourth one being deleted (because $\lambda_3 = 0$). The results of a few other 2-parameter procedures were $\Pi(\lambda_0 = 0.029, \lambda_1 = -2.0) = 12.60$ nm^3, $\Pi(\lambda_0 = 0.061, \lambda_1 = -4.4) = 12.70$ nm^3, to mention those with almost as good

results. Single-parameter procedures with λ_2 and λ_3 delivered significantly smaller values: $\Pi(\lambda_2 = 0) = 7.21$ and $\Pi(\lambda_3 = 0) = 0.82$ nm^3, but the other two were quite good: $\Pi(\lambda_0 = 0.78) = 11.73$ (same as the 2-parameter procedure with λ_0 and λ_3) and $\Pi(\lambda_1 = -1.27) = 11.26$ nm^3. The dependences $\Pi(\lambda_1)$, $\delta_{12}(\lambda_1)$, and $\mu_{12}(\lambda_1)$, for $\lambda_3 = 0$, are given in Figs. 5 and 6.

From the above results we conclude that it is essential in the optimization procedure to vary at least one of the parameters (λ_0 or λ_1) that correspond to "active" states. Variation of other parameters may help improving the final result, though not very much, while varying only the parameters corresponding to "inactive" states leads to highly underoptimized results. Finally, we note that introducing even more parameters by multiple deletion and restoring of the same state also did not give any improvements.

4. Conclusion

The multiparameter SUSYQM-based method of optimizing the QW potential shape was proposed. It starts with an rather arbitrarily chosen initial potential (just satisfying the resonance conditions) and modifies its shape isospectrally, in a manner controlled by a number of free scalar parameters. These are varied to find the QW profile which maximizes the property of interest. The method was explored on the example of maximizing the second order nonlinear susceptibility relevant for the optical rectification. Finally, the guidelines for this procedure are given.

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