Quantum-Well Tridiagonal: A Qualitative Comprehension of Optoelectronics Nanotechnology

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Abstract

A simple effective algorithm ("**QUANTUM-WELL TRIDIAGONAL**") for studying the essential features, causalities, and applicabilities of an optoelectronics nanoheterointerfacial generic quantum well (QW) is outlined in terms of transforming the pertinent initial Schroedinger equation into a normalised Sturm – Liouville one and, ultimately, into an eigensystem concerning a specific tridiagonal matrix. A qualitative comprehension of optoelectronics nanotechnology basics is, thus, envisaged to be offered.

1. Introduction

The investigation of semiconductor heterointerfaces is a prominent subject of ongoing research in view of the crucial importance which they possess for the functionality of numerous optoelectronic microdevices [1 – 6].

For more than two decades, the designing strategy of wavefunction-engineering [7] has systematically been giving birth to an admirable wealth of innovative semiconductor devices offering a high degree of tunability in their optoelectronic performance.

Celebrated pioneering microelectronic heterostructures of the kind have been the Bloch oscillator [8, 9], the resonant tunnelling double heterodiode [10], the hot electron tunnelling transistor [11], and the revolutionary quantum cascade LASER [12, 13].

In the present Paper, a simplifying effective algorithm (**QUANTUM-WELL TRIDIAGONAL**) for studying the essential features, causalities, and applicabilities of an optoelectronics nanoheterointerfacial generic quantum well (QW) is outlined in terms of transforming the pertinent initial Schroedinger equation into a normalised Sturm – Liouville one and, ultimately, into an eigensystem concerning a specific tridiagonal matrix. A qualitative comprehension of optoelectronics nanotechnology basics is, thus, envisaged to be offered.

2. QUANTUM-WELL TRIDIAGONAL Algorithm

With respect to the generic situation of a conductivity electron being hosted by the quantum well (QW) of potential energy profile U(x) against the growth axis coordinate x within a conventional semiconductor nanodevice heterointerface, the pertinent Schrödinger equation, concerning the electron de Boglie time – independent wavefunction ψ (x) and taking into account the spatial variation m^* (x) of the carrier effective mars, reads:

$$-\frac{d}{dx}\left[\frac{\hbar^2}{2m^*(x)}\frac{d\psi(x)}{dx}\right] + U(x)\,\psi(x) = E\,\psi(x), \quad (1)$$

with E being the allowed energy eignevalue conjugate to each physically meaningful wavefunction ψ(x), solving (1) and vanishing asymptotically at infinities,

and $\hbar$ being Planck's action constant divided by 2π.
Performing, now, an independent variable transformation, namely,

$$\chi \equiv \alpha\, x^* \,\mathrm{Arctanh}\,(\xi) \leftrightarrow \varphi(\xi) \equiv \psi[x(\xi)], \quad (2)$$

we obtain in place of (1) the Sturm – Liouville differential equation

$$\frac{d}{d\xi}\left[\mu(\xi)\frac{d\varphi(\xi)}{d\xi}\right] - \upsilon(\xi)\varphi(\xi) + \lambda\sigma(\xi)\,\varphi(\xi) = 0, \quad (3)$$

under the boundary conditions

$$\varphi(-1) = 0 \;\&\; \varphi(+1) = 0, \quad (4)$$

with functions $\mu(\xi), \upsilon(\xi)$ and $\sigma(\xi)$ in the new dimensionless variable ξ (belonging to the universal interval [-1, +1]) defined as

$$\mu(\xi) \equiv \frac{1}{\alpha}(1-\xi^2)\frac{m_o}{m^*[x(\xi)]}, \quad (5)$$

$$\upsilon(\xi) \equiv \frac{2\alpha}{1-\xi^2}\frac{U[x(\xi)]}{E^*}, \quad (6)$$

$$\sigma(\xi) \equiv \frac{2\alpha}{1-\xi^2}, \quad (7)$$

and dimensionless new, "reduced energy", eigenvalue λ defined as

$$\lambda = \frac{E}{E^*}, \quad (8)$$

where E^* denotes a convenient energy scale

$$E^* \equiv \frac{\hbar^2}{m_o x^{*2}} \equiv 1\,\mathrm{eV}, \quad (9)$$

rendering the characteristic confinement length x^* entering the independent variable transformation (2) after the dimensionless scale factor α equal to 2.76043 $\overset{0}{A}$, m_o giving the electron rest mass.

For converting the Sturm – Liouville differential equation concerning the nanoheterointerface two-dimensional electron gas (2DEG) transformed wavefunction φ(ξ) into a linearised system of difference equations, we employ the numerical approximation

$$\frac{d}{d\xi}[\,\mu(\xi)\frac{d\phi(\xi)}{d\xi}] \to \frac{1}{k}[\mu_{i+\frac{1}{2}}(\frac{\phi_{i+1}-\phi_i}{k}) - \mu_{i-\frac{1}{2}}(\frac{\phi_i-\phi_{i-1}}{k})], \quad (10)$$

in which the computational (nodal and interstitial, respectively) grid points ξ_n (whence $f_n \equiv f(\xi_n)$ with f standing for function φ, μ, υ, and σ, as the case might be) are chosen as

$$\xi_i = -1 + ik \ (i = 0,1,2,\ldots, N+1),$$
$$\xi_{i\pm\frac{1}{2}} = \xi_i \pm \frac{k}{2} \ (i = 1,2,\ldots, N+1), \quad (11)$$

for a uniform grid spacing

$$k = \frac{1-(-1)}{N+1} = \frac{2}{N+1}, \quad (12)$$

and for which the adjoint boundary conditions become

$$\phi_0 = \phi(\xi_0) = \phi(-1) = 0$$

&

$$\phi_{N+1} = \phi(\xi_{N+1}) = \phi(-1 + (N+1)\frac{2}{N+1}) = \phi(+1) = 0. \quad (13)$$

The Schrödinger equation eigenvalue problem is, thus, approximated by the system of finite difference equations

$$\{\alpha_i\phi_{i-1} + \beta_i\phi_i + \gamma_i\phi_{i+1} = -k^2\Lambda\phi_i ; i = 1,2,\ldots, N\} \quad (14)$$

or, equivalently, in tridiagonal matrix rows form,

$$\{\sum_{j=1}^{N}\{[\alpha_i\delta_{i-1,j}+\beta_i\delta_{i,j}+\gamma_i\delta_{i+1,j}]\phi_j\}=-k^2\Lambda\phi_i\ ;i=1,2,...,N\} \quad (15)$$

($\delta_{i,j}$ being the Kronecker delta), with the sets of coefficients $\alpha_i, \beta_i, \gamma_i$ defined as

$$\alpha_i \equiv \frac{\mu_{i-\frac{1}{2}}}{\sigma_i}, \gamma_i \equiv \frac{\mu_{i+\frac{1}{2}}}{\sigma_i}, \beta_i \equiv -(\alpha_i + \gamma_i + \frac{k^2 v_i}{\sigma_i}); i=1,2,...,N, \quad (16)$$

and Λ denoting the approximation to the exact reduced energy eigenvalue λ (E_q. (15)), produced by the constructed numerical algorithm and expected to more closely converge to it with increasing number N of computational grid nodal points ξ_i utilised.

The treatment has, therefore, evolved into the matrix eigenvalue problem

$$\{\sum_{j=1}^{N}\{\Lambda_{i,j}\phi_j\}=-k^2\Lambda\phi_i; i=1,2,...,N\}, \quad (17)$$

with the N-th order square tridiagonal matrix

$$\{(\Lambda_{i,j}\ ; j=1,2,...,N); i=1,2,,...,N\}$$

defined by

$$\Lambda_{i,j} \equiv \alpha_i\delta_{i\text{-}1,j} + \beta_i\ \delta_{i,j} + \gamma_i\ \delta_{i+1,j}. \quad (18)$$

Indeed; the opposite of the eignvalues of matrix $\{\Lambda_{i,j}\}$ divided by k^2 give Λ, the approximations to the heterointerface wavefunction exact reduced energy eigenvalues λ, thus computing (E_q.(15)) the allowed QW 2DEG subband energies $E = \lambda E^*$. Obviously, given that the general Strum – Liouville system (10) may admit an infinite sequence of eigenvalues λ, the finite succession of N eigenvalues Λ for algorithmic matrix $\{\Lambda_{i,j}\}$ provides the numerical approximations to only the N lowest true reduced energy eigenvalues λ, a slightly lessening approximation sufficiency for the last higher order computed eigenvalues being algorithmically probable. On the other hand, the N determined, Strum – Liouville eigenvectors $|\varphi(\xi)>$ conjugate to these numerical eigenvalues Λ unveil through transformation (9) the quantum mechanically allowed wavefunctions ψ (x) for the 2DEG dwelling within the nanodevice heterointerface QW and underlying the crucial optoelectronic effects exhibited by the generic semiconductor nanostructure. In particular, such a determination of the nanoheterointerface 2DEG wavefunction may lead to the computation of its entailed penetration length into the nanodevice neighbouring energy barrier layer, thus facilitating the prediction of 2DEG mobility behaviour parameterised by the order of wavefunction excitation and, furthermore, the consideration of quantum mechanical tunnelling transmission probability for conductivity electrons escaping the heterointerface and travelling through the nanodevice – by virtue of a normal transport mechanism advantageously exploitable, especially at nanoelectronic cryogenic ambient temperatures [14 – 22].

For studying the applicability of the herewith proposed optically pumped dual resonant tunnelling LASER action unipolar charge transport mechanism we now consider an indicative generic semiconductor nanoheterostructure based on the conventional Al_xGa_{1-x} As/GaAs material system.

In particular, we employ two totally asymmetric – both in the spatial width and in the energetic barrier height –, communicating through an intervening barrier layer, approximately rectangular quantum wells, both formulated within (different portions of) the GaAs semiconductor: The front QW [F] of spatial width 96 ^{o}A and energetic barrier height 221 meV, contained between a surface $Al_{0.3}$ $Ga_{0.7}$ As slab and the inter – QW communication barrier layer, and the back QW [B] of growth axis extension 162 ^{o}A and energetic confinement hill 204 meV, spanning the region between the inter – QW communication barrier layer and a botton Al $_{0.33}$ $Ga_{0.67}$ As slab. The intervening, inter – QW communication barrier layer may non – exclusively be regarded as the succession (either abrupt or graded) of two rather equithick sublayers of $Al_{0.3}$ $GA_{0.7}$ As and $Al_{0.33}$ $Ga_{0.67}$ As.

In this manner, the partially localised conductivity electron eignestates accommodated by the couple of communicating QWs in the model application under study correspond to the energy eigenvalues (measured within each QW from its energetic bottom upwards): E (**If>**) = 32 meV, E (**If '>**) = 136 meV – for the front QW fundamental and first excited bound state, respectively, - and E (**Ib>**) = 14 meV, E (**Ib'>**) = 55 meV, and E (**Ib''>**) =121 meV – for the back QW fundamental, first excited, and second excited bound state, respectively.

Notably, against this predicted energy eigenvalue configuration, the fundamental back QW eigenstate **Ib>** elevated by 14 meV over the back QW energetic botton finds itself well aligned with the conjugate fundamental eigenstate **If>** of the front QW raised above its QW energetic botton by an amount corresponding to the inter – QW energetic bottom discrepancy plus, about, the former fundamental eigenstate **Ib>** height over its local QW bottom.

In an analogous manner, the uppermost bound eigenstates of the two communicating QW, emerge aligned, as the difference in the height of each over its local QW bottom almost cancels the energetic height asymmetry of the two QW bottoms.

The determinable intersubband transition (ISBT) effective dipole lengths, furthermore, demonstrate the oscillator strengths supporting the different ISBT events, whereas the LASER action population inversion predicted would lead to the device stimulated optical gain.

3. Application

Within the extension of the typical nanoheterointerface (NHI), the energy-band bendings of the energetic-barrier portion and the conductive channel are being determined by its neighbouring (ionised-impurity) electric-charge density and overall field (with any effective non-built-in one incorporated). Thus, on the one hand the 2DEG confined sublevels are quantum-mechanically calculable and, on the other, the thermodynamic- equilibrium requirement mirrors an ultimate uniform Fermi-energy level throughout the nanoheterojunction to a realistic sheet-concentration of QW two-dimensional electrons.

At each instance of such dynamic equilibrium, the energetic top of actually filled NHI 2DEG states aligns with the uniform Fermi-level operative:

$$\mathrm{E}_0 + \frac{\zeta}{\rho} = \mathrm{E}_F \qquad (19)$$

,

with E_F being exactly the Fermi-energy level, E_0 being the energetic bottom of the 2DEG fundamental subband (considered as the only one occupied near the electric quantum limit, approached by conventional NHIs primarily functioning at ambient temperatures in the vicinity of absolute zero), ζ being the instantaneous 2DEG sheet- concentration within the NHI QW, and ρ being the theoretical two-dimensional per-unit-area (normal to the QW spatial extension) density of states accessible to conductivity electrons having their normal wavevector-component quantised, given in the parabolic approximation by

$$\rho = \frac{m^*}{\pi\hbar^2} \qquad (20)\ ,$$

where m* denotes the conductivity-electron effective mass at the NHI QW fundamental subband, and $\hbar$ Planck's action constant divided by 2π.

Commonly, modulation doping of the epitaxially composed nanodevice embeds a heavily dense donor-distribution within the wider-bandgap-semiconductor part of the NHI being established, with the donor energy-level getting located sufficiently deep –with reference to the bandgap profile- for the Fermi level to be plausibly regarded as pinned to it and remaining there (with, effectively, negligible rate of change) for the entire regime of quantum-limit-like nanodevice functioning. Such a

Fermi-level immunity against evolving cumulative photonic intake (tantamount to increasing 2DEG population being hosted by the NHI QW) by the nanoheterostructure would be sustainable through a mechanism successively lowering the 2DEG fundamental sublevel E_0 (as well as the first excited sublevel, which nevertheless would not be participating in the hosting of QW conductivity electrons as always lying over the Fermi-energy demarcation) within the QW being commensurately broadened whilst keeping its energetic depth dictated by the invariable NHI conduction-band discontinuity.

Considering, therefore, the dynamics of energy-level positions against regulated successive photon-doses being absorbed by the probed NHI, we obtain through partial differentiation of (19) with respect to the instantaneous cumulative photonic dose δ:

$$\frac{\partial E_0}{\partial \delta} + \frac{1}{\rho}\frac{\partial \zeta}{\partial \delta} = \frac{\partial E_F}{\partial \delta} \cong 0 \qquad (21),$$

or,

$$\frac{\partial E_0}{\partial \delta} = -\frac{1}{\rho}\frac{\partial \zeta}{\partial \delta} \qquad (22),$$

providing the photonic dose-rate of evolution of the 2DEG fundamental-eigenstate sublevel E_0 in terms of the experimentally traceable photon-dose-rate of augmentation of the 2DEG areal density ζ within the QW of the monitored NHI.

In this sense, (4) is following the photodynamics of the evolving photonic modification of the NHI fundamental-eigenstate, during the procedure of successive intakings of appropriate photon-transmissions: To each experimentally measurable Δζ(δ) for the augmentation of the 2DEG sheet-concentration ζ (with respect to its pre-illumination initial value ζ_d) consequent upon some instantaneous total photon-dose δ, the respective eigenstate-sublevel shift $\Delta E_0(\delta)$ (away from its dark locus E_{0d}) drawn by this cumulative dose δ is awaited, through to (4), to be:

$$\Delta E_0(\delta) = -\frac{1}{\rho}\Delta\zeta(\delta) \qquad (23)$$

.

This predicted gradual photolowering of NHI eigenstate-subband bottom is interpretable as quantum-mechanically compatible with previous studies of ours approximating the modification of a generic nanodevice's conductive-channel extension as positively linearly proportional to the respective 2DEG areal-concentration alteration

The finite-difference-method algorithm is incorporated in the following procedure, repeatedly performed for each successive experimental cumulative photon-dose δ:

1. Extraction from predictive-scheme Eq.(23) of the expected 2DEG fundamental-sublevel photolowering conjugate to experimentally measured 2DEG sheet-density persistent photoenhancement (PPE) driven by current total photonic intake.

2. Deduction of current 2DEG fundamental sublevel by subtraction of the absolute value of current fundamental-sublevel photolowering from sublevel dark (prior to exposure to photonic doses) locus.

3. Iterative applications of the algorithm with respect to a sought-for 2DEG QW spatial width compatible with the respective fundamental-eigenstate sublevel predicted for the current cumulative photonic dose. The entailed potential-energy profile U(x ; δ) is simplifyingly simulated by a rectangular one, of energetic depth always expressible by the NHI conduction-band discontinuity and resting on the boundaries of the photowidened QW spatial extension. Thus, the parametrisation of the QW potential-energy profile by total photonic intake δ is effected through letting a simulative fixed-energetic-depth rectangular model-QW expand spatially at a rate induced by each current intaken cumulative photon-dose.

4. Once the iterative algorithm has converged for the optimum QW spatial width conjugate to the current total photonic intake, the adjoint 2DEG fundamental-eigenstate wavefunction $\psi_0(x ; \delta)$ is obtained, thus exhibiting its traceable penetration-length [22] into the NHI energetic-barrier part.

Therefore, tracing the fundamental-eigenstate penetration-length in the optimum wavefunction $\psi_0(x ; \delta)$ obtained by convergence (with respect to the optimum QW width compatible with predicted photoredefined eigenstate locus) of the iterative algorithm for each total photon-dose intaken, we manage to map its photodynamics. Indeed, initial results connected to the current photodynamics model give fundamental-sublevel photolowering by about 22 - 28 meV and reduced (over dark value) fundamental-eigenfunction penetration length photoshrinkage to about 64 - 66 % , as the cumulative absorbed photon-dose scans six orders of magnitude over the responsivity threshold, for three distinct sample families monitored.

4. Conclusion

A simplifying effective algorithm (**QUANTUM-WELL TRIDIAGONAL**) for studying the essential features, causalities, and applicabilities of an optoelectronics nanoheterointerfacial generic quantum well (QW) is outlined in terms of transforming the pertinent initial Schroedinger equation into a normalised Sturm – Liouville one and, ultimately, into an eigensystem concerning a specific tridiagonal matrix. A qualitative comprehension of optoelectronics nanotechnology basics is, thus, envisaged to be offered.

Furthermore, in an application performed from such a comprehension perspective, the photodynamics of the NHI 2DEG eigenstate by absorption of regulated successive photon-doses is studied for the generic case of a conventional nanoheterodiode, in terms of the 2DEG fundamental-sublevel eigenenergy's correlation with respective 2DEG areal density, versus instantaneous cumulative photonic intake. The scheme is applicable to the experimental photoresponse of typical modulation-doped nanoheterodiodes and also allows for the deduction of the NHI 2DEG wavefunction penetration-length, as computed through an iterative algorithm converting the Sturm – Liouville differential equation concerning the NHI 2DEG transformed wavefunction into a tridiagonal-matrix eigenvalue-problem.

The predicted trend, thus, of evolving red photoshift for the NHI eigenstate sublevel would be compatible with a proceeding NHI QW-extension photowidening, on the one hand, and a NHI wavefunction penetration-length shrinking, on the other.

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