A QUALITATIVE COMPREHENSION OF NANO\PHOTONICS

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Abstract: - A simple effective algorithm (“QUANTUM-\WELL TRIDIAGONAL”) for studying the essential features, causalities, and applicabilities of a nanophotonics heterointerfacial 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 nanophotonics basics is, thus, envisaged to be offered.

Keywords: - Optoelectronics Nanotechnology, Nanophotonics, Nanointerface Quantum Well, Finite-Difference Algorithmic Modelling.
1. Introduction

The inspiration for the ingenious notion and ergonomic functionality of the photon has, in fact been triggered off by the challenge of comprehending in 1900 the experimentally measured blackbody radiation spectral distribution of energy density: Planck, on the one hand, assuming quantisation of the energy emitted by the walls of a radiation-confining cavity, introduced then energy quanta into the empirical pertinent formula; Rayleigh, on the other, proposed counting of the density of electromagnetic-radiation discrete modes (with respect to spatial volume and wavenumber interval), a quantity ultimately conceived and operationally utilised as the photon density of states \( D(\omega) = \omega^2/(\pi^2 c^3) \) (with \( \omega \) being the electromagnetic signal circular frequency and \( c \) being its vacuum phase-velocity).

A little afterwards, in 1905, Einstein employed inherent quantisation of light energy in his Nobel-winning interpretation of the Photoelectric Effect, by which a metal target shone upon by proper-wavelength illumination emits photoelectrons. Einstein, also, managed to reprove the blackbody-radiation spectral density formula by invoking the principle of precise balance between (stimulated) excitations and (both spontaneous and stimulated) de-excitations, regarding any couple of energy levels within the framework of an ensemble of discrete energy states pertaining to a set of quantum systems (Fabry-Perrot cavity atoms) maintaining in equilibrium with radiation. But it was in 1924 that Bose faced directly the blackbody radiation as an equilibrium gas of light quanta described by the (bosonic particle-relevant Bose-Einstein statistics) distribution function \( N(h\omega) = \left[e^{h\omega/(k_B T)} - 1\right]^{-1} \) (with \( k_B \) being Boltzmann thermodynamic constant and \( T \) being the Kelvin absolute temperature).

Born, Jordan and Heisenberg, furthermore, proposed in 1925 consideration of cavity-confined radiation in terms of elementary quantum oscillators with energy spectrum \( E(\omega_k) = h\omega_k (n_k + \frac{1}{2}) \), \( n = 0, 1, 2, 3, \ldots \), with \( n_k \) regarded as the number of quanta in a certain state designated by wavevector \( k \) and with a quantal zero-point energy term \( E_0 = (h/2) \sum_k \omega_k \). In the following year 1926, then, Schrödinger’s Equation for the de Broglie matter-wave
function was published, leading to the previous discrete radiation-quantum (photon) energy spectrum as now emerging through solution for a harmonic oscillator’s parabolic potential-energy quantum well: \( n_k \) number of photons in the \( k \)-mode of radiation (with the polarisation state additionally parametrisng each \( k \)-mode) and \( \hbar \omega_k \) energy portion per single photon.

Photonics is underlain by absorption, emission, generation, handling, and exploiting light, typically within the electromagnetic radiation spectrum range between 100 nm of the ultraviolet and 1,000 nm of the infrared – with the human visual perception focused upon the 400 – 700 nm optical interval.

Nanophotonics, now, with its recently formulating disciplinary autonomy, traces, interprets, and envisions nanotstructural spatial confinement – induced, often mystifying, modifications in light propagation and light-matter interaction. Nanophotonics, thus, as studying the essence and manifestations of confined electron de Broglie waves and confined light-wave photon flows, could be decomposed [23] into rather four categorical families of phenomena: Electron confinement effects on the optical properties of matter (semiconductors and dielectrics, in particular), light-wave confinement effects (in dielectric and photonic-crystal nanostructures), Quantum Optics of nanodevices (for the interaction operating between their resident electrons and their, under nanoconfinement, visitor and hosted light waves), and Nanoplasmonics concerning electron collective excitations at metal-dielectric nanointerfaces.

The investigation of semiconductor heterointerfaces, now, 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 nanophotonics 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 $\psi(x)$ and taking into account the spatial variation $m^*(x)$ of the carrier effective mass, reads:

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

with $E$ being the allowed energy eigenvalue conjugate to each physically meaningful wavefunction $\psi(x)$, solving (1) and vanishing asymptotically at infinities,

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

\[ \chi = \alpha x^* \text{Arctanh} (\xi) \leftrightarrow \varphi(\xi) = \psi[\chi(\xi)], \]  

(2)

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

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

(3)

and dimensionless new, “reduced energy”, eigenvalue \( \lambda \) defined as

\[ \lambda = \frac{E}{E^*}, \]

(8)

where \( E^* \) denotes a convenient energy scale

\[ E^* = \frac{\hbar^2}{m_o x^{*2}} = 1 \text{ eV}, \]

(9)

under the boundary conditions

\[ \varphi(-1) = 0 & \varphi(+1) = 0, \]

(4)

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

\[ \mu(\xi) = \frac{1}{\alpha} \left( 1 - \xi^2 \right) \frac{m_o}{m^* [x(\xi)]}, \]

(5)

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

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

$$\xi_i = -1 + ik \ (i = 0, 1, 2, \ldots, N + 1),$$

$$\xi_{i+1/2} = \xi_i \pm \frac{k}{2} \ (i = 1, 2, \ldots, N + 1),$$

(11)

for a uniform grid spacing

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

(12)

and for which the adjoint boundary conditions become

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

&

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

(13)

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

\[ \{\alpha_i\phi_{i-1} + \beta_i\phi_i + \gamma_i\phi_{i+1} = -k^2\Lambda\phi_i ; i = 1,2,\ldots,N\} \]

(14)

or, equivalently, in tridiagonal matrix rows form,

\[ \sum_{j=1}^{N} \{\alpha_i\delta_{i-1,j} + \beta_i\delta_{i,j} + \gamma_i\delta_{i+1,j}\phi_j\} = -k^2\Lambda\phi_i ; i = 1,2,\ldots,N \]

(15)

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

\[ \alpha_i = \frac{\mu_{i-\frac{1}{2}}}{\sigma_i}, \quad \gamma_i = \frac{\mu_{i+\frac{1}{2}}}{\sigma_i}, \quad \beta_i = -(\alpha_i + \gamma_i + \frac{k\nu_i}{\sigma_i}) ; i = 1,2,\ldots,N \]

(16)

and \(\Lambda\) denoting the approximation to the exact reduced energy eigenvalue \(\lambda\) (Eq. (15)), produced by the constructed numerical algorithm and expected to more closely converge to it with increasing number \(N\) of computational grid nodal points \(\xi_i\) utilised.

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

\[ \sum_{j=1}^{N} \{\lambda_{i,j}\phi_j\} = -k^2\Lambda\phi_i ; i = 1,2,\ldots,N \}, \]

(17)

with the \(N\)-th order square tridiagonal matrix

\[ \{\lambda_{i,j} ; j = 1,2,\ldots,N\} ; i = 1,2,\ldots,N \}

defined by
Indeed; the opposite of the eigenvalues of matrix \( \{ \Lambda_{ij} \} \) divided by \( k^2 \) give \( \Lambda \), the approximations to the heterointerface wavefunction exact reduced energy eigenvalues \( \lambda \), 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 \( \lambda \), the finite succession of \( N \) eigenvalues \( \Lambda \) for algorithmic matrix \( \{ \Lambda_{ij} \} \) provides the numerical approximations to only the \( N \) lowest true reduced energy eigenvalues \( \lambda \), 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 \( |\phi(\xi)> \) conjugate to these numerical eigenvalues \( \Lambda \) unveil through transformation (9) the quantum mechanically allowed wavefunctions \( \psi(\alpha) \) 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 \( \text{Al}_{x}\text{Ga}_{1-x}\text{As/GaAs} \) 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 Å 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 Å and energetic confinement hill 204 meV, spanning the region between the inter – QW communication barrier layer and a bottom 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 eigenvalue $\text{Ib}^>$ elevated by 14 meV over the back QW energetic bottom finds itself well aligned with the conjugate fundamental eigenstate $\text{If}^>$ of the front QW raised above its QW energetic bottom by an amount corresponding to the inter – QW energetic bottom discrepancy plus, about, the former fundamental eigenstate $\text{Ib}^>$ 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:

$$E_0 + \frac{\zeta}{\rho} = E_F$$

(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), \( \zeta \) being the instantaneous 2DEG sheet-concentration within the NHI QW, and \( \rho \) 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

\[
\rho = \frac{m^*}{\pi \hbar^2},
\]

(20),

where \( m^* \) denotes the conductivity-electron effective mass at the NHI QW fundamental subband, and \( \hbar \) Planck’s action constant divided by \( 2\pi \).

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 $\delta$:

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

or,

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

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 $\zeta$ 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 $\Delta \zeta(\delta)$ for the augmentation of the 2DEG sheet-concentration $\zeta$ (with respect to its pre-illumination initial value $\zeta_0$) consequent upon some instantaneous total photon-dose
ΔE₀(δ) = - \frac{1}{ρ} Δζ(δ)
(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 $U(x ; \delta)$ 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 $\delta$ 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 a photonics 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 nanophotonics 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
References