Schroedinger Treatment and Wavefunction Engineering of Nanophotonic Device Functionality

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Abstract: - A treatment, substantiating through Schroedinger equation transformation and analysis, and an underlying wavefunction-engineering are carried out towards studying the multipurpose regulation of nanophotonic device functionality.

Key-Words: - Optoelectronic and Photonic Nanodevices, Schroedinger Treatment of Quantum-Well Systems, Wavefunction Engineering in Nanodevices

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 treatment, substantiating through Schrödinger equation transformation and analysis, and an underlying wavefunction-engineering are carried out towards studying the multipurpose regulation of nanophotonic device functionality.

2 Schroedinger Treatment of Quantum-Well Nanodevice Functionality

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:

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

with $E$ being the allowed energy eigenvale 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,

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

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

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

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under the boundary conditions
\[ \phi(-1) = 0 \quad \& \quad \phi(+1) = 0, \quad (4) \]

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

\[ \mu(\xi) = \frac{1}{\alpha} \left(1 - \xi^2\right) \frac{m_0}{m^* |x(\xi)|}, \quad (5) \]

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

\[ \sigma(\xi) = \frac{2\alpha}{1 - \xi^2}, \quad (7) \]

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

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

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

\[ E^* = \frac{\hbar^2}{m_0 x_*^2} \equiv 1 \text{ eV}, \quad (9) \]

rendering the characteristic confinement length \( x^* \) entering the independent variable transformation \((2)\) after the dimensionless scale factor \( \alpha \) equal to \(2.76043 \text{ A}, m_0 \) giving the electron rest mass.

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

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

in which the computational (nodal and interstitial, respectively) grid points \( \xi_n \) (whence \( f_n = f(\xi_n) \) with \( f \) standing for function \( \phi, \mu, \nu, \) and \( \sigma \), as the case might be) are chosen as

\[ \xi_i = -1 + ik \quad (i = 0, 1, 2, \ldots, N + 1), \]

\[ \xi_{i+\frac{1}{2}} = \xi_i \pm \frac{k}{2} \quad (i = 1, 2, \ldots, N + 1), \quad (11) \]

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

\[ \phi_0 = \phi(\xi_0) = \phi(-1) = 0 \]

&

\[ \phi_{N+1} = \phi(\xi_{N+1}) = \phi(-1 + (N + 1)) = \phi(+1) = 0. \quad (13) \]

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

(15)

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

\[
\alpha_i = \frac{\mu_i}{\sigma_i}, \quad \beta_i = \frac{\mu_i}{\sigma_i}, \quad \gamma_i = -\left( \frac{\alpha_i + \gamma_i + \frac{2}{\sigma_i}}{\sigma_i} \right); \quad i = 1, 2, \ldots, N,
\]

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

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

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

(17)

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

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

defined by

\[
A_{i,j} \equiv \alpha_i \delta_{i-1,j} + \beta_i \delta_{i,j} + \gamma_i \delta_{i+1,j}.
\]

Indeed; the opposite of the eigenvalues of matrix \(\{A_{i,j}\}\) 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 eigenvectors \(\phi(\xi)\) conjugate to these numerical eigenvalues \(\Lambda\) unveil through transformation (9) the quantum mechanically allowed wavefunctions \(\psi(x)\) 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 \(\text{Al}_x\text{Ga}_{1-x}\text{As/GaAs}\) 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 \(\text{Å}\) and energetic barrier height 221 meV, contained between a surface \(\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}\) slab and the inter – QW communication barrier layer, and the back QW [B] of growth axis extension 162 \(\text{Å}\) and energetic confinement hill 204 meV, spanning the region between the inter – QW communication barrier layer and a bottom \(\text{Al}_{0.33}\text{Ga}_{0.67}\text{As}\) 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 \(\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}\) and \(\text{Al}_{0.33}\text{Ga}_{0.67}\text{As}\).

In this manner, the partially localised conductivity electron eigenstates 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): \( E (I_f^>) = 32 \text{ meV} \), \( E (I_f^>') = 136 \text{ meV} \) – for the front QW fundamental and first excited bound state, respectively, and \( E (I_b^>) = 14 \text{ meV} \), \( E (I_b^>') = 55 \text{ meV} \), and \( E (I_b^{''^>}) = 121 \text{ meV} \) – 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 \( I_b^> \) elevated by 14 meV over the back QW energetic bottom finds itself well aligned with the conjugate fundamental eigenstate \( I_f^> \) 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 \( I_b^> \) 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 Conclusion
A treatment, substantiating through Schroediner equation transformation and analysis, and an underlying wavefunction-engineering are carried out towards studying the multipurpose regulation of nanophotonic device functionality.

References: