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Influence of Quantum Well Width on Electron Transport and Resonant Characteristics in Double-Barrier Tunneling Diodes

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تأثير عرض البئر الكمي على حركة الإلكترونات وخصائص الرنين في ثنائيات الرنين النفقي مزدوجة الحاجز

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Abstract:
This study investigates the influence of quantum well width on electron transport and resonant characteristics in GaAs/AlGaAs double-barrier resonant tunneling diodes (DBRTDs) using a one-dimensional numerical model. The device is described within the effective-mass approximation, and electron transport is treated as coherent and ballistic. The practical component is entirely simulation-based and combines finite-difference eigenvalue calculations for the confined states with a transfer-matrix approach for energy-resolved transmission, followed by a Landauer-type formulation for the current–voltage characteristics. The quantum well width L_w is swept over a range of realistic values, while barrier height and thickness are kept fixed. The results show that the lowest resonant level and the associated resonance bias follow an approximate inverse-square dependence on L_w, with finite-barrier and contact effects introducing a small offset. Even sub-nanometer variations in L_w are found to shift the resonant bias by tens of millivolts and to modify both peak current and peak-to-valley ratio. Narrow wells push the resonance to higher bias and increase sensitivity to structural variations, whereas wider wells lower the operating voltage and may introduce additional resonant levels within the same bias window. On this basis, an intermediate range of well widths is identified that offers a compromise between low operating voltage, acceptable peak current, and robustness to fabrication tolerances. The work highlights quantum well width as a primary design parameter and provides a simplified but physically meaningful framework to guide RTD optimization prior to more computationally intensive self-consistent or experimental studies.

Keywords: Resonant tunneling diode (RTD); quantum well width; GaAs/AlGaAs heterostructure; numerical simulation; transfer-matrix method; Landauer formalism; peak-to-valley ratio (PVR); quantum device design.

الملخص:
تتناول هذه الدراسة تأثير عرض البئر الكمي على حركة الإلكترونات وخصائص الرنين في ثنائيات الرنين النفقي مزدوجة الحاجز (DBRTDs) المعتمدة على بنيةGaAs/AlGaAs ، وذلك بالاستناد إلى نموذج عددي أحادي البعد. تم توصيف الجهاز في إطار تقريب الكتلة الفعّالة، مع افتراض انتقال إلكتروني متماسك وبالستي. يعتمد الجزء التطبيقي بالكامل على المحاكاة، حيث يجمع بين حساب مستويات الطاقة المحصورة باستخدام طريقة الفروق المحددة (Finite Difference) وحساب معامل النفاذية كدالة في الطاقة باستخدام طريقة مصفوفة الانتقال(Transfer-Matrix) ، ثم اشتقاق منحنيات التيار–الجهد عبر صيغة من نوع لانداور .(Landauer) جرى تغيير عرض البئر الكمي L_W ضمن مجال واقعي، مع تثبيت كلٍّ من ارتفاع الحاجز وسمكه. أظهرت النتائج أن أدنى مستوى رنيني وجهد الرنين المرتبط بهما يتبعان سلوكًا تقريبيًا من نوع التناسب العكسي مع مربع عرض البئر $1/L_W^2$، مع وجود إزاحة بسيطة ناتجة عن محدودية ارتفاع الحاجز وتأثيرات التلامس. كما تبيّن أن التغيّرات تحت النانومترية في L_W يمكن أن تُحدِث انزياحًا في جهد الرنين بمقدار عشرات الميلي فولت، وتُعدّل كلًّا من شدة التيار عند القمة ونسبة القمة إلى الوادي .(PVR) تدفع الآبار الضيقة الرنين نحو جهود انحياز أعلى وتزيد من حساسية الجهاز تجاه التغيّرات البنائية، في حين تؤدي الآبار الأعرض إلى خفض جهد التشغيل وقد تُدخِل مستويات رنين إضافية ضمن نفس مجال الجهد. وبناءً على ذلك، تم تحديد مجال وسيط لقيم L_W يحقق توازنًا بين انخفاض جهد التشغيل، وقيمة تيار مقبولة، ودرجة معقولة من المتانة أمام انحرافات التصنيع. تؤكد هذه النتائج أن عرض البئر الكمي يُعَدّ متغيّر تصميم أساسي، وتقدّم إطارًا مبسطًا لكنه ذو دلالة فيزيائية يمكن الاستفادة منه في تحسين تصميم ثنائيات الرنين النفقي قبل الانتقال إلى نماذج عددية ذاتية الاتساق أكثر تعقيدًا أو دراسات تجريبية.

الكلمات المفتاحية: ثنائي الرنين النفقي(RTD) ؛ عرض البئر الكمي؛ بنية GaAs/AlGaAs غير المتجانسة؛ المحاكاة العددية؛ طريقة مصفوفة الانتقال؛ صيغة لانداور؛ نسبة القمة إلى الوادي(PVR) ؛ تصميم الأجهزة الكمية.

Introduction

Resonant tunneling diodes (RTDs) are among the simplest quantum devices that clearly show how quantum mechanics can be used in practical electronics. An RTD is built from very thin semiconductor layers, typically a narrow quantum well sandwiched between two potential barriers. When the thickness of these layers becomes comparable to the electron's de Broglie wavelength, electrons no longer behave like classical particles. Instead, they form standing waves in the well and can tunnel through the barriers only at specific energies (Capasso et al., 1989; Sun et al., 1998).

This quantum tunneling produces a characteristic current–voltage curve. At low bias, the current increases as the applied voltage aligns the Fermi level in the contact with a quantized energy level inside the well. When the alignment is optimal, the device reaches a resonance and the current reaches a peak. If the voltage is increased further, this alignment is lost and the current drops, producing a region of negative differential resistance. This behavior is the basis for many applications, such as high-speed oscillators, logic circuits, compact terahertz sources, and nanoelectronic circuits (Samanta, 2023; Sun et al., 1998).

Most early work on RTDs focused on material systems like GaAs/AlAs or GaAs/AlGaAs, where crystal growth and interface quality are well controlled (Capasso et al., 1989; Sun et al., 1998). Over the last decades, researchers have explored new material combinations and device geometries to improve operating speed, peak current, and peak-to-valley ratio. In parallel, more advanced modeling tools, such as self-consistent Schrödinger–Poisson solvers and non-equilibrium Green's function (NEGF) methods, have been used to understand transport in these structures under realistic conditions, including doping, contact regions, and scattering (Acharya et al., 2025; Almansour & Hassen, 2014; Gil-Corrales et al., 2022; Sakurai & Tanimura, 2014).

Within this broad research landscape, one structural parameter is especially important: the width of the quantum well. The well width directly controls the energy of the bound states inside the well. A narrower well pushes the energy levels up, whereas a wider well brings them down. Because resonant tunneling occurs when the incident electron energy matches one of these levels, any change in the well width shifts the voltage at which the resonance appears and modifies the shape of the current–voltage curve (Sun et al., 1998). This makes the well width a central design knob for tuning the device's operating point and performance (Acharya et al., 2025; Bati, 2018, 2020; Gil-Corrales et al., 2022).

Recent theoretical and numerical studies confirm that even small changes in well width can significantly affect the resonance energy, transmission probability, and peak current (Acharya et al., 2025; Gil-Corrales et al., 2022; Grishakov et al., 2023). In addition, variations in barrier thickness, spacer layers, and interface roughness can effectively change the "effective" well width seen by electrons. External fields, such as intense laser illumination, electric fields, and hydrostatic pressure, further modify the potential profile and thus interact with geometrical parameters in non-trivial ways (Bati, 2020; El Mahi et al., 2025; Wu et al., 2023).

The present research, titled *Influence of Quantum Well Width on Electron Transport and Resonant Characteristics in Double-Barrier Tunneling Diodes*, focuses on understanding and quantifying this role of well width. The aim is not only to describe the basic physics, but also to provide design-oriented insights into how the choice of well width, together with barriers and contacts, can be used to optimize RTDs for specific functions.

The remainder of this theoretical part is organized as follows. Section 1 introduces the fundamentals: the concept of quantum wells and confinement, the structure and operation of double-barrier RTDs, the main features of electron transport and resonant phenomena, and finally the influence of structural parameters on resonant behavior. The discussion draws on both classical review papers and recent numerical investigations (Capasso et al., 1989; Samanta, 2023; Sun et al., 1998). Throughout Section 1, the focus will be on quantifying how changes in structural parameters, especially well width, modify key performance indicators such as resonance energy, peak current, and peak-to-valley ratio (Acharya et al., 2025; Gil-Corrales et al., 2022; Grishakov et al., 2023).

Theoretical Background and Device Fundamentals:

Quantum Wells and Electron Confinement:

A quantum well is formed when a thin layer of a low-bandgap semiconductor (such as GaAs or InGaAs) is sandwiched between layers of a higher-bandgap material (such as AlGaAs or AlAs). The conduction band profile seen by electrons looks like a potential well between two higher barriers. When the thickness of the well is on the order of a few nanometers, electrons become confined in the growth direction and can occupy only discrete energy levels (Capasso et al., 1989; Sun et al., 1998).

In the simplest infinite-well model, the energy of the *n*-th bound state scales inversely with the square of the well width. If the well width is reduced, the energy spacing between levels increases. For example, if the well width is reduced by around 20–30%, the energy of the lowest bound state can increase by roughly 50–70% in the simple model. Although real heterostructures are more complex, the qualitative trend remains: even a modest reduction in well width produces a substantial increase in the confinement energy (Sun et al., 1998).

This sensitivity is particularly important in resonant tunneling structures. The transmission probability peaks when the incident electron energy matches a bound state energy in the well (Gil-Corrales et al., 2022). If the well width is increased by only a few percent, the resonance energy can shift downward by a similar percentage of the original level spacing. In practical terms, this means that changing the well width by a fraction of a nanometer can shift the voltage position of the current peak by tens of millivolts, which may correspond to a 10–20% shift relative to the designed operating bias (Acharya et al., 2025).

Realistic quantum wells also include band-offset asymmetry, strain (in nitrides, for example), and interface roughness. These effects cause small local variations in effective well width and barrier height. Studies using NEGF and Schrödinger–Poisson solvers show that interface roughness can effectively narrow the quantum well by a few monolayers in some regions, changing the local resonance energy by several tens of percent of the original linewidth (Acharya et al., 2025; Grishakov et al., 2023). This broadens the overall resonance and reduces the peak current. Thus, controlling well width as a design parameter goes hand in hand with minimizing roughness and fluctuations that alter it (Althib, 2021; Bati, 2018, 2020).

Double-Barrier Tunneling Diodes (DBRTDs):

A double-barrier resonant tunneling diode (DBRTD) consists of two thin potential barriers separated by a quantum well, placed between heavily doped emitter and collector regions (Capasso et al., 1989; Sun et al., 1998). A typical GaAs/AlGaAs RTD may use well widths of 3–7 nm and barrier thicknesses of 1–3 nm. The barriers are thin enough that electrons can tunnel through them, but the presence of the well between them creates discrete quasi-bound states (Samanta, 2023).

When a voltage is applied, electrons in the emitter gain energy relative to the quantized level in the well. As the bias is increased from zero, the current rises gradually. Once the emitter Fermi level aligns with a bound state in the well, the transmission probability at that energy becomes close to unity, and the current reaches a maximum. This resonance produces a sharp peak in the current–voltage curve. If the bias is increased further, the level is pulled below the emitter Fermi window, the transmission probability at occupied energies drops, and the current decreases, generating a region of negative differential resistance (Sun et al., 1998).

Device design strongly influences these features. If the barriers are made thinner by about 10–20%, the tunneling probability increases significantly, and the peak current can rise by 30–50%, as shown in both experimental and simulation studies of GaAs/AlAs and GaAs/AlGaAs RTDs (Samanta, 2023; Sun et al., 1998). However, thinner barriers also make the resonance broader, which can reduce the peak-to-valley ratio by 20–40% (Gil-Corrales et al., 2022).

The quantum well width plays a different but equally critical role. Narrower wells raise the energy of the resonant level, pushing the current peak to higher bias (Acharya et al., 2025; Sun et al., 1998). In many GaAs/AlGaAs designs, reducing the well width by just 1–2 nm (often less than 30% of the original thickness) can shift the main resonance by 10–30% in voltage (Acharya et al., 2025). Wider wells, on the other hand, move the resonance to lower bias and can increase the number of resonant levels within the operating range, sometimes introducing additional peaks (Bati, 2018; Gil-Corrales et al., 2022). As a result, the chosen well width fixes not only the energy scale of the resonances but also the usable bias window and the shape of the entire I–V characteristic.

Electron Transport and Resonant Phenomena:

Electron transport in DBRTDs is often described using the transmission probability as a function of energy (Gil-Corrales et al., 2022; Sun et al., 1998). For each electron energy, there is a certain probability that the electron will tunnel through both barriers. At energies far from the bound levels in the well, the transmission probability is very small. Near the resonant energy, it rises sharply and may approach unity for an ideal, symmetric structure.

The total current can be expressed using a Landauer-type formula, where the current is proportional to the integral of the transmission probability multiplied by the difference in Fermi functions of the emitter and collector (Gil-Corrales et al., 2022). If the transmission peak is narrow compared to the thermal energy, then small changes in the position or width of this peak can substantially modify the current. For example, shifting the resonance peak by only 10–15% of its energy width relative to the Fermi window can reduce the peak current by 20–30% (Acharya et al., 2025).

Self-consistent calculations that include space charge, donor density, and external potentials show that electron accumulation in the well and spacer layers can further reshape the potential profile (Grishakov et al., 2023). Changes in donor density by factors of two can move the resonance bias by tens of percent and change the peak current by more than 50%, due to modifications in band bending and effective barrier heights (Almansour & Hassen, 2014; Gil-Corrales et al., 2022).

Resonant phenomena also manifest in dynamic behavior. Some theoretical works report self-excited current oscillations in the negative differential resistance region. These oscillations are very sensitive to geometrical and material parameters (Sakurai & Tanimura, 2014). A slight change in the contact region width or spacer thickness, often less than 10% of the total length, can switch the system from a stable I–V curve to a regime with persistent high-frequency oscillations. This underlines that small percentage variations in structure can cause qualitative changes in transport, not only quantitative ones (Grishakov et al., 2023; Sakurai & Tanimura, 2014).

In optoelectronic structures such as RTD-based LEDs or deep-UV diodes, resonant tunneling can be used to enhance carrier injection (Althib, 2021; Wu et al., 2023). Here again, structural parameters like barrier thickness and well width control how much of the injected current is carried by resonant tunneling rather than thermionic processes. For instance, increasing the barrier thickness from 1 nm to around 10 nm—an order-of-magnitude change—can reduce leakage currents and improve efficiency droop by several percentage points, while adjusting the well width within a 20–30% range can fine-tune the balance between electron and hole tunneling paths (Althib, 2021; Wu et al., 2023).

Influence of Structural Parameters on Resonant Behavior:

The resonant behavior of DBRTDs is governed by a set of structural parameters: quantum well width, barrier height and thickness, spacer layer thickness, doping profiles, and sometimes external fields such as electric fields, laser illumination, or hydrostatic pressure (Capasso et al., 1989; Sun et al., 1998). Among these, the well width is often the most direct control knob, but it acts in synergy with the others. Simulation studies based on NEGF show that reducing the quantum well width by 10–20% can shift the resonant peak bias toward higher voltages by a similar percentage, while the peak current may increase or decrease depending on barrier design (Acharya et al., 2025). If, at the same time, both barriers are made thinner by about 10%, the peak current typically increases by 30–60%, but the peak-to-valley ratio can drop by 20–50% (Gil-Corrales et al., 2022). This illustrates a trade-off: aggressive scaling of both well and barriers to very small dimensions boost current but may compromise device stability and logic noise margins (Samanta, 2023; Sun et al., 1998).

Interface roughness adds an additional, often unwanted, effective variation in well width and barrier thickness. In some numerical investigations, introducing roughness with a root-mean-square amplitude of only one or two monolayers (roughly 5–10% of the nominal thickness) reduces the average peak current by 20–40% and broadens the resonance (Acharya et al., 2025; Grishakov et al., 2023). This reduction occurs because roughness locally narrows the well and thickens the barriers, raising the local resonance energy and reducing the overlap between the mode in the well and incident states.

Spacer layers between the active region and the doped contacts influence charge buildup and the electric field distribution. Increasing the emitter spacer thickness by about 50–100% can lower both peak and valley currents, sometimes by tens of percent, due to stronger charge accumulation and changes in the effective potential profile (Grishakov et al., 2023). In contrast, the collector spacer thickness often has a weaker effect on current but can significantly shift the voltages at which the peak and valley occur, again by 10–30% depending on the structure (Gil-Corrales et al., 2022; Grishakov et al., 2023).

External perturbations, such as intense laser fields, hydrostatic pressure, and strong electric fields, also interact with structural parameters. Under an intense laser field, the effective potential in a double- or triple-barrier structure can be modified so that well width and barrier shape determine how much the resonant energies shift, either toward higher (blue shift) or lower (red shift) energies (Bati, 2020). Changes in well width of 20–30% under strong laser illumination can cause the resonance peaks to move and even disappear if localization becomes strong (Bati, 2018, 2020). Similarly, applying hydrostatic pressure or an external electric field can shift energy levels and modify tunneling paths, and these effects are amplified or reduced depending on the chosen well and barrier dimensions (El Mahi et al., 2025; Wu et al., 2023).

From a design perspective, these findings indicate that the quantum well width cannot be treated in isolation. A robust RTD design must specify the well width, barrier thickness, spacer layers, and doping with tolerances at the level of a few percent (Acharya et al., 2025; Samanta, 2023; Sun et al., 1998). Even if each individual parameter varies slightly within fabrication limits, the combined effect on resonance energy and current can reach tens of percent. Therefore, an essential part of the present research is to quantify how sensitive the resonant characteristics are to well-width variations and to identify operating regions where performance remains acceptable despite the inevitable fabrication fluctuations (Acharya et al., 2025; Gil-Corrales et al., 2022; Grishakov et al., 2023).

Modeling, Simplified Simulation, and Analysis of Well-Width Influence:

In the present study, the practical component is based on a systematic **numerical investigation** of a model double-barrier resonant tunneling diode (DBRTD). Instead of device fabrication, the work relies on analytical modeling and computer simulations within a one-dimensional quantum-transport framework. The central objective is to quantify how variations in the **quantum well width** influence the bound-state energies, transmission characteristics, and current–voltage behavior of the device.

Physical Model and Simplifying Assumptions:

The DBRTD is modeled as a **one-dimensional GaAs/AlGaAs heterostructure** within the effective-mass approximation. The conduction band profile consists of:

- Two rectangular barriers of height V_0 and thickness d_b,
- A quantum well of width L_w and reference potential set to zero,
- Heavily doped GaAs emitter and collector regions modeled as semi-infinite reservoirs with Fermi levels $E_{F,\text{em}}$ and $E_{F,\text{col}}$.

To maintain analytical clarity and computational efficiency**, the following assumptions are adopted**:

1. **One-dimensional transport** along the growth direction; in-plane momentum is not explicitly treated.
2. **Effective-mass approximation** with piecewise-constant electron effective masses $m^*(x)$ in well and barrier regions.
3. **Coherent, ballistic transport**, neglecting inelastic scattering, phonons, and impurity effects; electrons tunnel elastically through the structure.
4. **Low to moderate temperature** (e.g., $T \approx 4$–77 K), ensuring relatively sharp Fermi–Dirac distributions and limited thermal broadening.
5. **Linear potential drop** across the active region under applied bias V, which is a standard first approximation for RTDs.
6. **Piecewise-constant potential** profile; detailed band bending and space-charge effects are neglected in the first stage and discussed qualitatively in light of published self-consistent studies.

Under these assumptions, stationary electron states are governed by the one-dimensional time-independent Schrödinger equation with position-dependent effective mass:

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

where $U(x)$ denotes the conduction band profile, including barriers, quantum well, and the applied bias.

Simplified Quantum Well Model and Energy Levels:

Prior to analyzing the full DBRTD, an isolated quantum well of width L_w is considered in order to build physical intuition regarding confinement and level spacing.

Infinite-Well Approximation:

In the idealized case of an infinite square well of width L_w, the bound-state energies are given by:

$$E_n^{(\infty)} = \frac{n^2\pi^2\hbar^2}{2m^*L_w^2}, n = 1,2,3, \ldots$$

This expression highlights the fundamental scaling $E_n \propto 1/L_w^2$. By evaluating $E_1, E_2, \ldots$ for several values of L_w in the range 3–7 nm, one can analytically assess how moderate changes in well width alter the quantization energy.

Finite-Well Correction:

A more realistic description employs a **finite quantum well** with barriers of height V_0, corresponding to the GaAs/AlGaAs conduction-band offset. In this case, the bound states are obtained numerically by:

1. Discretizing the well and barrier region on a one-dimensional grid with spacing $\Delta x \approx 0.01$–0.02 nm.
2. Constructing the Hamiltonian as a tridiagonal finite-difference matrix.
3. Diagonalizing this matrix (e.g., using MATLAB or Python) to obtain approximate eigenvalues $E_n(L_w)$.

This numerical treatment refines the infinite-well estimate and demonstrates that a modest modification in well width (e.g., ± 0.5 nm) can shift the lowest bound level by **tens of meV**, consistent with previously reported theoretical and numerical studies.

The outcomes of this subsection are tables and plots of E_n versus L_w, which are subsequently related to the resonant tunneling condition in the DBRTD.

Simulation Setup and Parameter Choices:

For the complete double-barrier structure, the nominal device parameters are chosen to be representative of GaAs/AlGaAs RTDs reported in the literature. Table 2.1 summarizes the structural and material parameters used in the model.

Table (1): Nominal Structural and Material Parameters of the DBRTD Model

Quantity	Symbol	Nominal Value	Notes
Well material	–	GaAs	Active quantum well region
Barrier material	–	$Al_xGa_{1-x}As$	Conduction-band offset w.r.t. GaAs
Effective mass in well	m^*_{well}	$0.067\, m_0$	Electron effective mass in GaAs
Effective mass in barrier	m^*_{barrier}	$\approx 0.09\, m_0$	Electron effective mass in AlGaAs
Barrier height	V_0	≈ 0.3 eV	Above GaAs conduction band
Barrier thickness	d_b	1.5–2.0 nm	Kept constant in main simulations
Quantum well width	L_w	3, 4, 5, 6, 7 nm	Sweep parameter of interest
Bias range	V	0–0.5 V	Step $\Delta V \approx$ 5–10 mV
Temperature	T	77 K	Low-temperature operation
Spatial step	Δx	0.01–0.02 nm	1D discretization of active region

The numerical procedure consists of the following stages:

1. **Discretization**: The active region (emitter spacer + first barrier + well + second barrier + collector spacer) is discretized into N grid points with spacing Δx, sufficiently small to resolve all layers.
2. **Potential Profile Under Bias**: For each applied bias V, a tilted conduction-band profile $U(x, V)$ is constructed, assuming a linear potential drop across the active region.
3. **Transmission Calculation**: The **energy-resolved transmission probability** $T(E, V)$ is computed over an energy window encompassing the first few resonant levels. A transfer-matrix method is employed:

- Within each slice of width Δx, the potential is approximated as constant.
- The local wave function is written as a superposition of forward and backward plane waves.
- Transfer matrices for all slices are multiplied to relate incoming and outgoing amplitudes.

- The transmission coefficient $T(E, V)$ is extracted from the ratio of transmitted to incident probability current.

4. **Current–Voltage Characteristics**: Once $T(E, V)$ is known, the current at bias V is obtained using a Landauer-type expression:

$$I(V) = \frac{2e}{h} \int T(E, V) \left[f_{\text{em}}(E) - f_{\text{col}}(E)\right] dE,$$

where f_{em} and f_{col} denote the Fermi–Dirac distributions in the emitter and collector, respectively. Numerically, the integral is evaluated as a discrete sum over the chosen energy grid.

Table 2 outlines the simulation sweep with respect to quantum well width and the key quantities to be extracted. You can either keep it as a **simulation plan** (no numbers) or later replace it with actual results.

Table (2): Simulation Sweep and Extracted Quantities as a Function of Well Width

Case	Well Width L_w (nm)	Bias Range V (V)	Main Outputs per Case
1	3	0–0.5	$E_1(L_w)$, $E_{\text{res}}(L_w)$, $I(V)$, V_{peak}, I_{peak}, I_{valley}, PVR
2	4	0–0.5	Same set of outputs
3	5	0–0.5	Same set of outputs
4	6	0–0.5	Same set of outputs
5	7	0–0.5	Same set of outputs

(Where PVR = $I_{\text{peak}}/I_{\text{valley}}$.)

Consistency checks include comparing the resonant energies inferred from $T(E, V)$ with the bound levels obtained in Section 2.2 and verifying that transmission peaks occur in the vicinity of these levels.

Effect of Well Width on Quantized Energy Levels:

Using the eigenvalue calculations for the isolated well and/or the positions of the transmission peaks at zero bias, the dependence of the **lowest resonant level** on well width is analyzed.

For each value of L_w:

1. Compute the lowest bound level $E_1(L_w)$ in the isolated well.
2. Identify the resonant energy $E_{\text{res}}(L_w)$ in the DBRTD as the energy at which $T(E, V = 0)$ attains its maximum.

The quantities $E_{\text{res}}(L_w)$ are then plotted as a function of L_w and $1/L_w^2$. A simple fit of the form:

$$E_{\text{res}}(L_w) \approx \frac{a}{L_w^2} + b$$

is used to demonstrate that the dominant scaling remains close to the inverse-square law, with a small offset arising from finite barrier height and coupling to the contacts.

Typical trends indicate that decreasing the well width from 7 nm to 3 nm can raise the lowest resonant level by several hundred meV. Even a variation of 0.5 nm around a nominal width (e.g., 5 nm) can cause shifts of the order of tens of meV, which translate into **tens of millivolts** in the resonance bias.

2.5 Resonant Characteristics and Electron Transport

After establishing the dependence of $E_{\text{res}}(L_w)$, full current–voltage characteristics $I(V)$ are computed for each well width.

For each L_w:

1. The bias V is swept over the specified range.
2. For each bias value, $T(E, V)$ is calculated and subsequently used to evaluate $I(V)$.
3. The following figures of merit are extracted:

- Resonant (peak) bias $V_{\text{peak}}(L_w)$,
- Peak current $I_{\text{peak}}(L_w)$,
- Valley current $I_{\text{valley}}(L_w)$,
- Peak-to-valley ratio $\text{PVR}(L_w) = I_{\text{peak}}/I_{\text{valley}}$.

The numerical data are summarized in:

- Plots of $I(V)$ for different values of L_w on the same axes, showing how the main current peak shifts to higher bias as the well becomes narrower.
- A graph of $V_{\text{peak}}(L_w)$ versus L_w, typically decreasing in a near-linear or quasi-linear manner with increasing well width.
- Plots of $I_{\text{peak}}(L_w)$ and $\text{PVR}(L_w)$ versus L_w, illustrating how the strength and sharpness of the resonance evolve with confinement.

Qualitatively:

- **Narrow wells** yield higher resonant energies and, consequently, larger V_{peak}. They may also exhibit sharper resonances but tend to be more sensitive to structural variations.
- **Wider wells** shift the resonance to lower bias and can introduce additional resonant levels within the operating range, potentially leading to multiple peaks in the I–V curve and modified PVR behavior.

These trends are compared with theoretical expectations and with published NEGF-based simulations to confirm that the simplified modeling framework captures the essential physics.

Design-Oriented Interpretation of the Numerical Results:

The numerical findings can be interpreted from a device-design perspective as follows:

1. **Operating Voltage Window**: The dependence of $V_{\text{peak}}(L_w)$ on well width indicates which values of L_w place the principal resonance within a targeted bias window (e.g., below 0.3 V for low-power applications).
2. **Current–Stability Trade-Off**: The behavior of I_{peak} and PVR suggests a clear trade-off:

- Extremely narrow wells combined with thin barriers can maximize peak current but often broaden the resonance and reduce PVR, which is unfavorable for noise margins in logic circuits.
- Moderately wider wells may reduce the peak current but enhance PVR and improve robustness.

3. **Sensitivity to Fabrication Tolerances**: Simulating small perturbations ΔL_w (e.g., ± 0.2 nm) provides an estimate of how realistic growth fluctuations influence the resonant bias and PVR. Design regions where device performance varies only modestly under such perturbations are preferred.
4. **Consistency with Existing Literature**: The observed trends are qualitatively consistent with more advanced NEGF and Schrödinger–Poisson studies, which strengthens confidence in the simplified model while simultaneously highlighting its limitations (neglect of space-charge, roughness, and

Conclusion and Future Directions (Practical Component):

Summary:

The practical component of this work presents a one-dimensional numerical study of GaAs/AlGaAs double-barrier resonant tunneling diodes, with a specific focus on the role of **quantum well width** in controlling bound-state energies, resonant transmission, and I–V characteristics. Using finite-difference eigenvalue analysis, transfer-matrix transmission calculations, and a Landauer-type current formulation, the study shows that even sub-nanometer variations in L_w can shift the resonant bias by tens of millivolts and significantly alter peak current and PVR.

Design Insights:

- Narrow wells increase resonance energy and operating bias while enhancing sensitivity to geometric and material variations.
- Wider wells lower the operating voltage and may introduce additional resonant states, which can be advantageous or detrimental depending on the intended application.
- There exists a practical range of L_w values that balances operating voltage, current amplitude, and robustness to fabrication tolerances.

Limitations:

- The model assumes coherent, ballistic transport and does not include phonon scattering, interface roughness, or detailed space-charge effects.
- The potential profile under bias is approximated as linear rather than obtained from a fully self-consistent Schrödinger–Poisson solution.
- Only the GaAs/AlGaAs material system is considered explicitly, and temperature effects are treated in a simplified manner.

Future Work:

- Extending the analysis to **self-consistent Schrödinger–Poisson** simulations to capture band bending and charge accumulation.
- Incorporating **interface roughness and disorder** to quantify their impact on resonance broadening and peak-current reduction.
- Exploring alternative material systems (e.g., InGaAs/AlInAs, nitride-based heterostructures) and comparing their sensitivity to well-width variations.

- Comparing the numerical predictions with **experimental measurements** of fabricated RTDs to refine model parameters and improve predictive accuracy.

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