

Scattering Rate Modeling in Semiconductor Quantum Wells and Quantum Cascade Lasers Using the 8-band $\mathbf{k} \cdot \mathbf{p}$ Formalism

by

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Author's Declaration

This thesis consists of material all of which I authored or co-authored: see Statement of Contributions included in the thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners. I understand that my thesis may be made electronically available to the public.

Statement of Contributions

Jiarun Bai was the sole author for Chapters 1, 2, and 4 which were written under the supervision of Dr. Dayan Ban and were not written for publication. This thesis consists of one manuscript written for publication. The following is an exception to sole authorship of material:

Research presented in Chapters 3:

This research was conducted at the University of Waterloo under the supervision of Prof. Dayan Ban. Prof. Ban and Dr. Emmanuel Dupont proposed the idea of fitting intersubband scattering lifetime measured from pump-probe experiments by 8-band $k \cdot p$. Dr. Emmanuel Dupont and Rebecca Mac's previous work established the $k \cdot p$ scattering calculation framework. Jiarun Bai applied this framework to simulate real-world quantum well structures, fit the pump-probe experimental data, and performed data collection and analysis. Jiarun Bai drafted the manuscript, and all authors provided intellectual input and assisted with revisions.

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Abstract

Accurate modeling of electron scattering is critical for understanding and optimizing carrier transport in semiconductor heterostructures such as quantum wells (QWs) and quantum cascade lasers (QCLs). In this thesis, we present a comprehensive study of scattering rate calculations using an advanced 8-band $k \cdot p$ formalism that incorporates nonparabolic band dispersion, multiband coupling, and k -dependent wavefunctions. This approach allows for precise modeling of subband structures and associated scattering mechanisms, such as longitudinal optical (LO) phonon, impurity, interface roughness (IFR), and alloy disorder (AD) scattering, which strongly influence electron lifetimes and optical transition rates in QCLs.

There are mainly two parts of this work. The primary objective of the first part work is to determine the interface roughness (IFR) and alloy disorder (AD) scattering parameters (Λ, Δ, V_{AD}) by fitting simulated electron subband scattering rates using the 8-band $k \cdot p$ model to pump-probe measurements for three InGaAs/AlGaAs quantum well samples. This fitting process, although is not sufficient to uniquely determine the AD, IFR parameters, gives a narrow range of those parameters, and serves to validate the accuracy of the 8-band $k \cdot p$ formalism. By only using 1-band model, the scattering rate is overestimated by $\sim 66\%$ in a QW tuned at $\lambda_{21} \sim 5 \mu\text{m}$, while using the 8-band model, a good agreement with the experimental data is obtained by properly choosing the aforementioned parameters. The reason this fitting is insufficient to narrow down those parameters to single value is due to the inherent time resolution of the pump-probe experiments, and the fact that alloy disorder and interface roughness scattering are processes of the same nature. To find the exact value of those parameters, one possible way would be associating this method with other material characterization techniques, such as ultra-high vacuum scanning tunneling microscope or electron tomography. Above all, this analysis confirmed the cruciality to consider not only the correct dispersion but also the k -dependent band-mixing effect.

The second part then extended to InAs/AlSb-based QCL structures to investigate the k -dependent confinement effect. When the wavevector k increases from zero, the shape of the wavefunctions will become more concentrated in one quantum well. This phenomenon, neglected in previous studies, directly affect the form factor in Fermi's Golden Rule and consequently has a significant impact on the transition rate. Two QCL structures are simulated with the same model in the first part. The wavefunctions and dispersion relations for each subband are calculated using 8-band $k \cdot p$ formalism. The primary focus is placed on the photon transition levels, with the higher energy state referred as the Upper Lasing State (ULS) and the lower energy state as the Lower Lasing State (LLS). In the simulation, the pair of subbands whose energy separation most closely matches the experimental photon

energy is selected as the ULS and LLS. The ULS is fixed at $k = 0$, while the LLS is evaluated at various wavevector values k . The qualitative change of the LLS wavefunction with increasing k directly demonstrate the confinement of wavefunction caused by the higher k value. The corresponding quantitative change is also shown by a defined parameter called static dipole, which measures the spatial separation between the expectation values of the ULS and LLS wavefunctions. Since the ULS remains fixed at $k = 0$, the separation change is caused by the LLS alone, therefore, is an effective indicator for the LLS confinement effect. This study further underscores the necessity of incorporating both k -dependent wavefunctions and nonparabolicity when calculating scattering rates. What's more, it further underscores the importance of incorporating k -dependent wavefunctions in accurate scattering rate calculations.

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Dedication

For my family and friends, who always stood by me.

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Chapter 1

Introduction

The advancement of modern technologies such as high-speed communication[4], IR imaging and sensing[5, 6], and energy harvesting [7] all rely heavily on the development of semiconductor heterostructures. Controlling how electrons move and interact at the nanoscale is key to achieving efficient and tunable operation. Among these, Quantum Cascade Lasers (QCLs) represents a sophisticated class of devices, engineered to emit light by guiding electrons transit through a series of quantum wells and barriers. Accurate modeling of electron transport in QCLs is essential for the design and optimization of modern optoelectronic devices. The computationally efficient rate equation and density matrix methods are the most commonly used electron transport modeling nowadays. The accuracy of these methods are directly influence by the carrier scatterings rate calculation. This introduction outlines the key scattering processes relevant to QCLs, the importance of accurate band structure modeling, and the motivation for adopting advanced 8-band $\mathbf{k} \cdot \mathbf{p}$ approaches in this work.

1.1 Significance of scatterings

Quantum Well (QW) structures, which are formed by sandwiching narrow band gap materials between two wider band gap barriers, are fundamental building blocks in modern optoelectronic devices due to their ability to confine carriers and discretize energy levels through quantum confinement[8, 9]. Among the many applications of QWs, QCLs stand out as a prime example of how engineered subband structures can be utilized to achieve an efficient and tunable light source, particularly in the mid-infrared and terahertz spectrum[10, 11]. Unlike conventional diode lasers that operate via interband transitions, QCLs utilize conduction band intersubband transitions. Fig. 1.1 shows the operation principle of a three-level two-well QCL is presented to demonstrate the operation principle. The operation of a QCL relies critically on how electrons transport between different pairs of subbands.

In QCLs and similar heterostructures, realistic electron transport modeling requires precise treatment of scattering mechanisms. For example, a common approach to modeling QCL operation is through the use of the rate equations or its generalized version – the density matrix[12]. These equations are based on the principle that the population of electrons in a given subband is determined by the balance between incoming and outgoing scattering transitions. Consequently, the accuracy of rate equation modeling is strongly dependent on the precision with which scattering rates are calculated.

The electron net scattering rate relies on four key mechanisms - longitudinal optical (LO) Phonons, ionized impurities (IMP), interface roughness (IFR), and alloy disorder (AD) scatterings[13, 14]. LO-phonon scattering is caused by the interaction between elec-

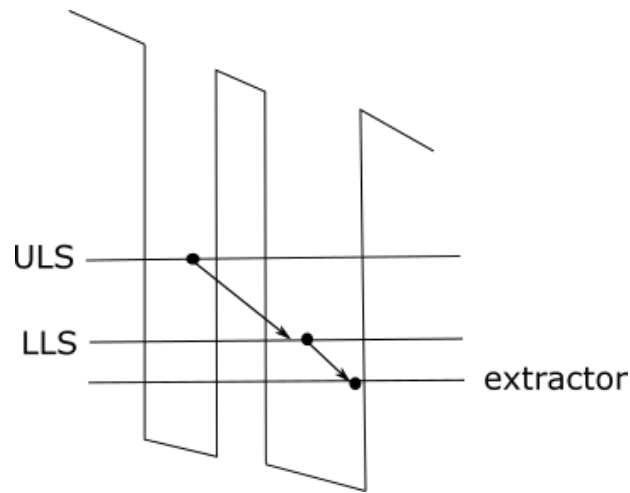


Figure 1.1: Simplified conduction-band diagram of a three-level two-well QCL structure, illustrating electron transitions from the upper lasing state to the lower lasing state and subsequently to the extractor state. Ideally, the transition from ULS to LLS would be purely radiative, however, in reality, nonradiative scatterings like LO phonon, impurity scatterings, etc will compete with the desired transitions. What's more, unwanted parasitic nonradiative transitions may also occur directly from ULS to the extractor or even to other subbands not shown on the diagram.

trons and LO phonons, which are quantized vibrations of atoms in a crystal lattice. Longitudinal means the atoms in the lattice vibrate along the direction of the wavevector, and optical refers to the displacements of neighboring atoms are in opposite phase[15]. While LO-phonon scattering is effectively used in QCLs as a depopulation route, in THz QCLs this very mechanism also acts as a major non-radiative loss channel, severely limiting room-temperature operation[16, 17]. One common approach to reduce the LO-phonon scattering between the upper and the lower lasing state is to make the transition diagonal, therefore the overlap between the wavefunctions can be reduced. Ionized impurity scattering, often referred to simply as impurity scattering, occurs when an electron is deflected by charged impurities within the crystal lattice. Impurity scattering can be significantly reduced by placing dopants in the barrier rather than the active region. Since if the electron density near the impurities is low, then electrons are less likely to be deflected by them, thereby reducing scattering. Another technique to reduce impurity scattering is to use “modulation doping” instead of “uniform doping”[18]. The IFR scattering refers to the disruption of electron motion caused by irregularities or fluctuations at the interfaces between different semiconductor layers[15]. These imperfections arise during the epitaxial growth process and lead to local variations in the potential landscape experienced by the electrons. Due to the nanoscale dimensions of QCL structures[19, 20, 21] (some layer thicknesses can be as small as a few monolayers), minor deviations at the interfaces(mean height ≈ 0.3 nm, in-plane correlation length, 7.3 nm)[14] can lead to significant alternations in the electronic potential profile, thereby impacting transition rates of electrons. Last but not least, alloy disorder scattering occurs when electrons are scattered by local compositional fluctuations. In other words, atoms are arranged perfectly in an ideal

periodic alloy crystal, however, in reality, atoms are randomly distributed and can cause local variations in potential profile. The scattering rate between subbands is computed using Fermi's Golden Rule, where the matrix elements are derived from the eigenstates of the multiband k·p Hamiltonian. In this framework, the accuracy of subband energies and wavefunctions directly governs the precision of predicted scattering rates.

1.2 Significance of band structure modelings

Accurate band structure modeling is essential because scattering rates are typically calculated using the Fermi's Golden rule which depends on the matrix element $\langle \psi_i | H_{perturb} | \psi_f \rangle$ and a energy conservation term, therefore it is extremely sensitive to subband wavefunction shapes and subband energy dispersions[15]. Small errors in calculated subband energies or wavefunction can lead to large deviations in predicted scattering rate. For instance, LO-phonon emission from an excited state will be highly efficient only if the subband separation nearly equals E_{LO} (the LO phonon energy) so that a resonant phonon can be emitted[22, 23]. Likewise, diagonal designs in QCLs [24, 25] and k-dependent confinement effects[13] demonstrate that the wavefunction shapes can determine the confinement or localization of carriers.

Common approaches for modeling band structures include the nearly free electron (NFE) model, tight-binding (TB) model, pseudopotential method, density functional theory (DFT), and the k·p method [26, 27, 28]. In the NFE model, a set of free-electron plane waves is used as basis, the weak lattice periodic potential is added as a perturbation to the free one-electron Schrodinger Equation. While this model can help to explain band

gap formation and work reasonably well for simple metals since electrons in metal are free to move, it is far too crude for semiconductors or systems where electrons are confined or localized. The tight-binding model, on the other hand, assumes electrons are tightly bound to atoms and only have a weak interaction with neighboring sites. It uses atomic orbitals (s-orbital, p-orbitals...) as the basis and is suitable for systems with strong covalent bonding or localized states. However, TB tends to be less accurate for conduction bands in III-V semiconductors, which have a more delocalized s-like character. Moreover, the accuracy of TB in modeling heterostructures is limited by the complexity of choosing suitable basis sets and coupling parameters. This makes it challenging to use TB for simulating extended states and delocalized wavefunctions across multiple wells in QCLs. With some complications (using more complicated atomic basis, and including second nearest neighbors), TB is proven to be able to model the energy band of heterostructures [29]. In the pseudopotential method, instead of treating the crystal potential as a perturbation, it introduces a weak pseudopotential to replace the strong, rapidly varying (especially near the core region) real potential. Density functional theory offers an ab initio framework by approximating the many-body electron problem in terms of electron density rather than wavefunctions. Although DFT is powerful and widely used for bulk material properties and interface modeling, it has significant limitations when applied to QCL structures, and the major drawback is that it is computationally expensive for large superlattices or layered heterostructures with dozens of quantum wells. Thus, DFT is generally impractical for large-scale systems.

In contrast to the limitations of the aforementioned approaches, the $\mathbf{k}\cdot\mathbf{p}$ method offers a computationally efficient and physically insightful framework for modeling the band struc-

ture of semiconductors, particularly in heterostructures [30, 15, 31, 28]. The $\mathbf{k} \cdot \mathbf{p}$ method arises naturally from the symmetry properties of the crystal and Bloch's theorem. In a periodic lattice, electronic wavefunctions can be written in the Bloch form. By inserting this form into the Schrodinger equation and expanding around a high-symmetry point such as the Brillouin zone center Γ , one obtains a perturbed Hamiltonian where the perturbation terms are proportional to $\mathbf{k} \cdot \mathbf{p}$, giving rise to the $\mathbf{k} \cdot \mathbf{p}$ method. The extension of $\mathbf{k} \cdot \mathbf{p}$ from bulk materials to heterostructures is pretty straightforward with the help of the envelope approximation.

Table 1.1: Comparison of common band-structure modeling methods.

Method	Strengths	Limitations	Main Applications
Nearly Free Electron (NFE)	Simple to implement.	Too crude for semiconductors	Basic metal structures.
Tight-Binding (TB)	Good for localized states.	Less accurate for conduction bands.	Covalent bonded materials.
Density functional theory (DFT)	Accurate for bulk/interfaces.	Computationally expensive for big heterostructures.	bulk/interfaces
$k \cdot p$	Efficient; More physically understandable.	Worse for far from expansion point.	Bulk; Envelope approximation for heterostructures.

1.3 Motivation and Research Objectives

Despite the advantage of $\mathbf{k} \cdot \mathbf{p}$ method mentioned above, typical implementation tends to over simplify to a one band (only conduction band), or three band model (conduction band, light hole band, and split-off band). This simplification either ignores the band-mixing effects caused by the valence bands, which, in other words, neglecting the nonparabolicity, or only forces the resulted wavefunction to be constrained at the bandedge, therefore, does not respect the momentum conservation for scattering processes.

For instance, Ref.[32] considers the nonparabolicity, however, ignored the wavefunction's k -dependency and the multiband-mixing effects. Ref.[33] proposes an advanced density matrix QCL transport model using a three-band Kane Hamiltonian, however, they tend to use a simplified dispersion and the eigenfunctions are only considered at $k=0$. Fig. 1.2 summarizes the discussion above and highlighted the main focus of this thesis.

None of them takes the k -dependency of wavefunctions into consideration. In a recent paper[13], our team pointed out the necessity of consider simultaneously: 1) A nonparabolic dispersion 2) a multi-band (8-band) scattering matrix element, and 3) k -dependent eigenfunctions within this matrix element. Fig.1.3 shows a comparison between ours and commonly used $\mathbf{k} \cdot \mathbf{p}$ methods. The following chapters detail the theoretical underpinnings, numerical methods, and experimental validation used to assess its effectiveness.

The goal of this project is to: (1): validate an 8-band $\mathbf{k} \cdot \mathbf{p}$ model developed within our research group by fitting the experimental pump-probe measurements of quantum well structures. (2): Demonstrate the k -dependent confinement effects resulted by including k -dependent wavefunctions.

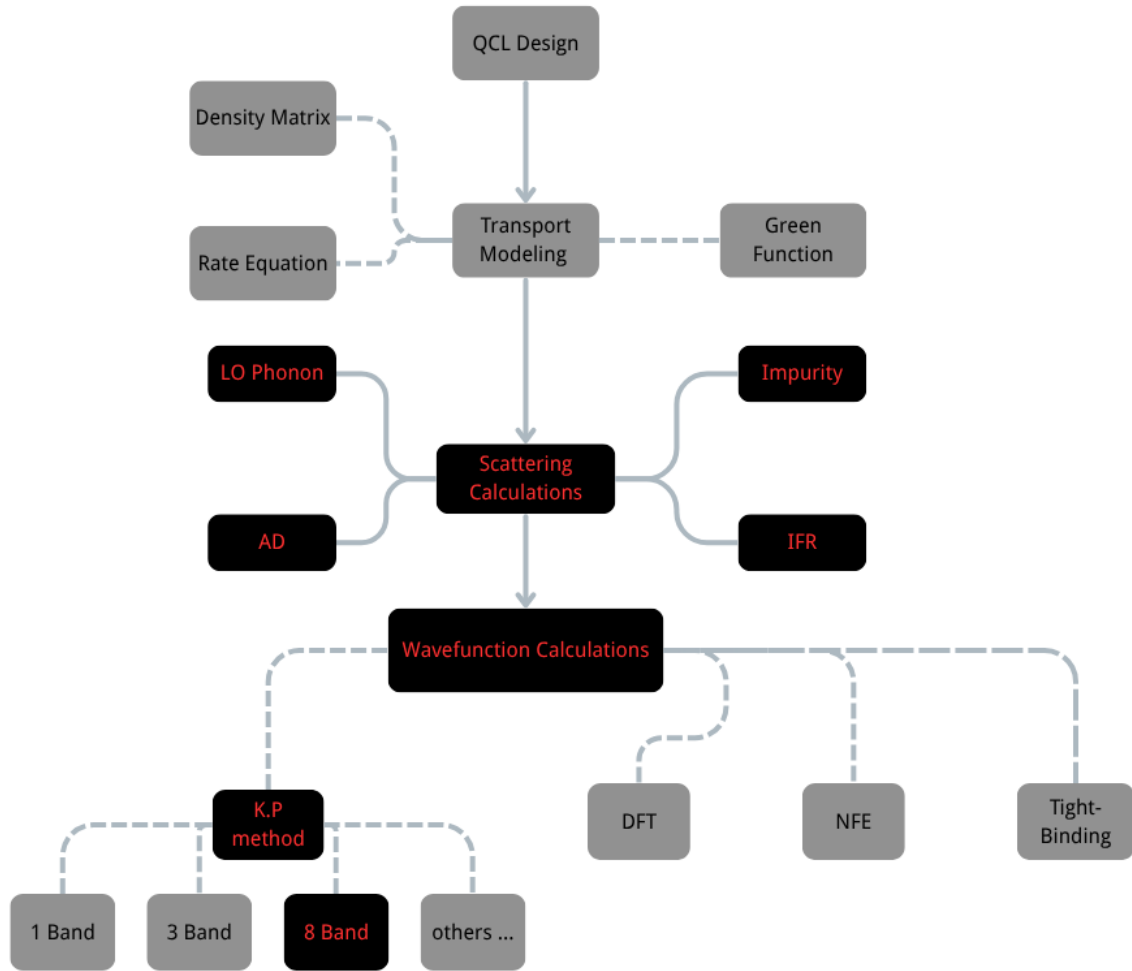


Figure 1.2: The black background with red font highlights the specific focus areas of this thesis. Dashed lines indicate alternative methods that could be employed at each stage, while solid lines represent the different components or aspects encompassed within a given step. The direction of the arrows reflects the logical or functional dependence between the connected elements.

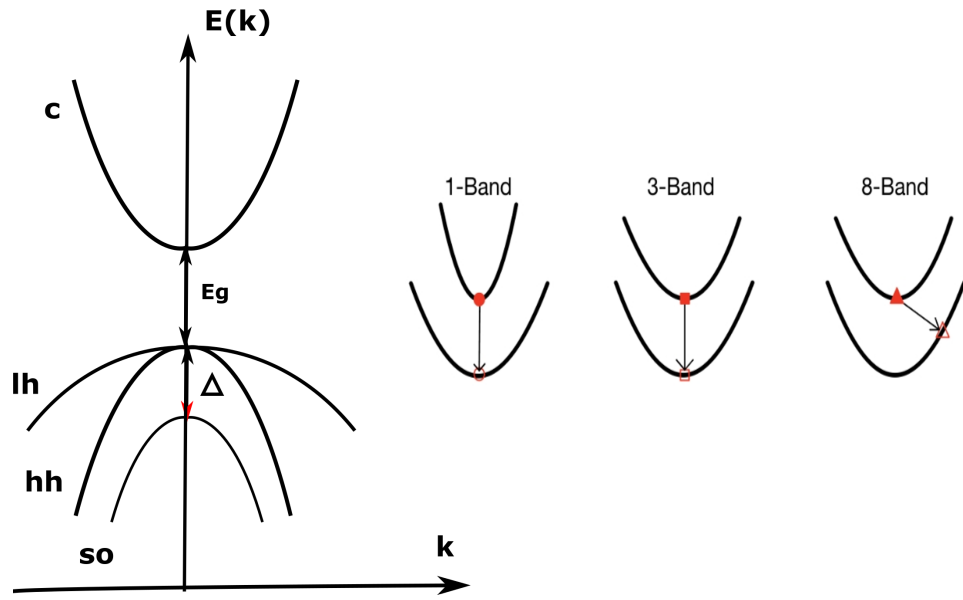


Figure 1.3: The 1-Band model only consider the conduction band and the resulted wavefunctions are fixed at $k=0$. The 3-Band model includes light-hole and split-off band, however, the wavefunctions are still fixed at $k=0$. The 8-band model considers the light-hole, heavy-hole, split-off, and conduction band plus their spin and also allows k to vary away from zero

The scientific significance of this work lies in advancing the theoretical framework used to model electrons scattering in QCLs by rigorously incorporating multiband mixing, non-parabolicity, and $\mathbf{k}$ -dependent wavefunction. These elements are often neglected or only partially considered in conventional models, resulting in inaccurate scattering rate predictions. Since the QCL device operation is extremely sensitive to scatterings, improved modeling can lead to the design of devices with higher wall-plug efficiency, extended temperature range, and tailored emission spectra.

1.4 Thesis Organization

- Chapter 2 discuss the analytical and numerical model implementation for the 8-band $\mathbf{k} \cdot \mathbf{p}$ model and the scattering rate calculation within that framework.
- Chapter 3 applied the $\mathbf{k} \cdot \mathbf{p}$ model to three Quantum Wells (QWs). The scattering rates are computed and fitted to the experimental transition rate obtained from pump probe experiments, with the aim of narrowing down the IFR, AD parameters range. This process not only constrained the key material parameters but also verified the validity of our 8-band $\mathbf{k} \cdot \mathbf{p}$ model and highlighted the necessity of using this comprehensive model.
- Chapter 4 applied the $\mathbf{k} \cdot \mathbf{p}$ model on InAs-based Quantum Cascade Laser (QCLs) to demonstrate the $\mathbf{k}$ -dependent confinement effect. The probability function of the final electronic state (the lower lasing state in the QCL design) and the static dipole were calculated over a range of kinetic energies, providing both qualitative and quantitative

insights into how confinement evolves with increasing k -values.

- Chapter 5 summarizes the contribution of this thesis and discusses future work.

Chapter 2

Theoretical Background

2.1 Overview of the $\mathbf{k} \cdot \mathbf{p}$ Method

The $\mathbf{k} \cdot \mathbf{p}$ method is a perturbative approach used to approximate band structures near high-symmetry points in the Brillouin zone, typically the Gamma points ($\mathbf{k}=0$). As early as the mid-1950s, Luttinger and Kohn pioneered a systematic framework for the $\mathbf{k} \cdot \mathbf{p}$ method[\[34\]](#). Their work generalized the effective mass equation to the case of degenerate bands, resulting in a set of coupled Schrodinger equations, which is later known as the LK model. This allowed for the accurate treatment of triply degenerate valence band maxima and non-central band extrema in indirect bandgap materials. Almost simultaneously, Dresselhaus, Kip, and Kittel experimentally validated the multiband $\mathbf{k} \cdot \mathbf{p}$ model through cyclotron resonance measurements of electrons and holes in silicon and germanium. Their findings demonstrated the model's effectiveness in explaining the anisotropy of heavy-hole and

light-hole effective masses. This model is later known as the DKK model [35]. Both models aim to describe the coupling and anisotropic dispersion of the degenerate valence bands at the Γ point. Despite differences in formulation, the two models describe the same underlying physics and are mathematically equivalent under proper transformation [28]. Building on earlier developments, E. O. Kane extended the k·p method in 1957 to describe the band structure of narrow-gap III–V semiconductors such as InSb, leading to a multi-band model that explicitly includes the coupling between conduction and valence bands [36]. The Kane model revealed important features of narrow-gap materials, such as nonparabolic conduction bands and spin splitting, laying the groundwork for later multi-band k·p models. Meanwhile, the introduction of the Envelope Function Approximation (EFA) allowed bulk k·p models to be adapted to heterostructures, including quantum wells and superlattices, making the k·p method a cornerstone in modern semiconductor band structure calculations [37, 38].

For application in bulk materials, the $\mathbf{k} \cdot \mathbf{p}$ method builds on Bloch's theorem, which expresses the wavefunction as:

$$\psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}) \quad (2.1)$$

where $u_{n\mathbf{k}}(\mathbf{r})$ has the periodicity of the lattice. Substituting this form into the Schrödinger equation $H(0) = \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r})$, we obtain:

$$H(\mathbf{k})u_{n\mathbf{k}} = E_n(\mathbf{k})u_{n\mathbf{k}} \quad (2.2)$$

with

$$H(\mathbf{k}) = H(0) + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} \quad (2.3)$$

Here, the $\mathbf{k} \cdot \mathbf{p}$ term represents first-order perturbation due to the crystal momentum, and the final term is the free-electron-like kinetic energy correction. To solve the eigenvalue problem, $u_{n\mathbf{k}}$ is expanded in a finite basis of zone-center Bloch functions $u_{m0}(\mathbf{r})$ (eigenstates of $H(0)$), leading to a matrix representation of the Hamiltonian. This formalism allows direct computation of $E_n(\mathbf{k})$ and effective masses.

2.2 2-Band Simple Example

To illustrate how the matrix formulation of the $\mathbf{k} \cdot \mathbf{p}$ method yields energy dispersion and effective mass, let us consider a simple two-level system involving a conduction band state $|c\rangle$ and a valence band state $|v\rangle$, which are eigenstates of the unperturbed Hamiltonian $H(0)$. We expand the perturbed state $u_{n\mathbf{k}}$ as:

$$u_{n\mathbf{k}} = c_c |c\rangle + c_v |v\rangle \quad (2.4)$$

Substituting this expansion into the Schrödinger equation $H(\mathbf{k})u_{n\mathbf{k}} = E_n(\mathbf{k})u_{n\mathbf{k}}$, we can derive the matrix elements. For example:

$$H_{11} = \langle c | H(\mathbf{k}) | c \rangle = \langle c | H(0) | c \rangle + \langle c | \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} | c \rangle + \langle c | \frac{\hbar^2 k^2}{2m_0} | c \rangle \quad (2.5)$$

which simplifies to:

$$H_{11} = E_c + \frac{\hbar^2 k^2}{2m_0} + \langle c | \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} | c \rangle \quad (2.6)$$

, where E_c is the conduction band energy.

The last term typically has the value zero, $\langle c | \mathbf{k} \cdot \mathbf{p} | c \rangle = 0$, and this can be rigorously justified using group theory. In the case of zincblende (ZB) crystals, the conduction band edge state $|c\rangle$ transforms according to the irreducible representation Γ_1 , corresponding to an s -like orbital [27]. The momentum operator $\mathbf{p}$, being a vector operator, transforms as Γ_{15} . The term $\langle c | \mathbf{k} \cdot \mathbf{p} | c \rangle$ involves a matrix element of the form $\langle \Gamma_1 | \Gamma_{15} | \Gamma_1 \rangle$, which is nonzero only if the identity representation Γ_1 appears in the decomposition of the direct product $\Gamma_{15} \otimes \Gamma_1$. However, using the properties of direct products, this reduces to Γ_{15} , which does not contain the identity representation Γ_1 . Therefore, by group-theoretic selection rules, the matrix element $\langle c | \mathbf{p} | c \rangle$ must vanish. For matrix element H_{22} , although $\langle v | \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} | v \rangle$ is not forced to be zero by the selection rule, we can still argue it will vanish since $\mathbf{p}$ has odd parity, and $|v\rangle$ has the same parity. Similarly, using the group theory selection rule, we can determine the only non-zero terms for the off-diagonal matrix elements are $\langle c | \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} | v \rangle$ and $\langle v | \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p} | c \rangle$. In the end, we obtain the matrix form of the Hamiltonian:

$$H(\mathbf{k}) = \begin{pmatrix} E_c + \frac{\hbar^2 k^2}{2m_0} & \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p}_{cv} \\ \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p}_{vc} & E_v + \frac{\hbar^2 k^2}{2m_0} \end{pmatrix} \quad (2.7)$$

To find the energy dispersion, we solve the secular equation:

$$\det(H(\mathbf{k}) - EI) = 0 \quad (2.8)$$

The determinant yields:

$$[E_c + \frac{\hbar^2 k^2}{2m_0} - E][E_v + \frac{\hbar^2 k^2}{2m_0} - E] - \left(\frac{\hbar}{m_0}\right)^2 (\mathbf{k} \cdot \mathbf{p}_{cv})^2 = 0 \quad (2.9)$$

Solving this quadratic equation in E gives two energy branches:

$$E_{\pm}(\mathbf{k}) = \frac{E_g + \frac{\hbar^2 k^2}{m_0}}{2} \pm \sqrt{\left(\frac{E_g + \frac{\hbar^2 k^2}{m_0}}{2}\right)^2 + \left(\frac{\hbar}{m_0}\right)^2 (\mathbf{k} \cdot \mathbf{p}_{cv})^2} \quad (2.10)$$

This expression shows how the conduction and valence bands become mixed due to the momentum coupling $\mathbf{p}_{cv}$, and how the bands deviate from simple parabolic shapes. For small $\mathbf{k}$ (near the Gamma point), we can expand the square root and approximate the conduction band energy as:

$$E_c(\mathbf{k}) \approx E_g + \frac{\hbar^2 k^2}{2m^*} \quad (2.11)$$

where the effective mass m^* is given by:

$$\frac{1}{m^*} = \frac{1}{m_0} + \frac{2|\mathbf{p}_{cv}|^2}{m_0^2 E_g} \quad (2.12)$$

This result reveals a key insight of the $\mathbf{k} \cdot \mathbf{p}$ method: the effective mass is modified by interband coupling, and becomes smaller (i.e., the band becomes more dispersive) when the coupling is strong or the bandgap is small. This explains the reduced effective mass in narrow-gap semiconductors like InSb or HgCdTe. This two-band example can be extended to multiple bands (such as the Kane 8-band model), which enables a much more accurate description of materials with strong band mixing, such as III-V semiconductors

and quantum well heterostructures.

2.3 Kane's Model

Kane's model represents a quasi-degenerate perturbative approach to multiband electronic structure modeling near the Brillouin zone center (Γ -point), and they extend the Dresselhaus-Kip-Kittel (DKK) [28] formulation by explicitly incorporating the conduction band and, in the more complete version, the effects of spin-orbit coupling. These models are widely used in the simulation of narrow-gap semiconductors and quantum heterostructures due to their ability to reveal the physics of band mixing and k-dependency. The 4-band Kane model consists of the lowest conduction band state and the three topmost valence band states: Conduction band(Γ_{6c}), Valence bands (Γ_{15v}) $|X\rangle, |Y\rangle, |Z\rangle$. This 4-band model captures the non-parabolicity caused by the interband coupling between the conduction and valence bands, and is often used as a minimal model for semiconductors where spin-orbit coupling is weak. The 8-band Kane model is an extension of the 4-band model that includes spin-orbital interaction, which is critical for accurate modeling of III-V semiconductors, especially in narrow-gap or strained systems [39]. For convenience, a new basis set is formed by the linear combination of $|S\rangle, |X\rangle, |Y\rangle, |Z\rangle$ states to diagonalize the total angular momentum $\mathbf{J} = \mathbf{L} + \boldsymbol{\sigma}$ and its projection $\mathbf{J}_z$, and they are noted as follow:

$$i|S \uparrow\rangle, \left|\frac{3}{2}, \frac{1}{2}\right\rangle, \left|\frac{3}{2}, \frac{3}{2}\right\rangle, \left|\frac{1}{2}, \frac{1}{2}\right\rangle, i|S \downarrow\rangle, \left|\frac{3}{2}, -\frac{1}{2}\right\rangle, \left|\frac{3}{2}, -\frac{3}{2}\right\rangle, \left|\frac{1}{2}, -\frac{1}{2}\right\rangle \quad (2.13)$$

Using these basis along with the Hamiltonian¹, $H = \frac{\mathbf{p}^2}{2m_0} + V(\mathbf{r}) + \frac{\hbar^2 \mathbf{k}^2}{2m_0} + \frac{\hbar \mathbf{k} \cdot \mathbf{p}}{m_0} + \frac{\hbar}{4m_0 c^2} (\boldsymbol{\sigma} \wedge \nabla V) \cdot \mathbf{p}$, the matrix representation of the 8-Band Kane Hamiltonian can be derived:

$$\begin{pmatrix} E_0 & -\sqrt{\frac{2}{3}}Pp_z & Pp_+ & \sqrt{\frac{1}{3}}Pp_z & 0 & -\sqrt{\frac{1}{3}}Pp_- & 0 & -\sqrt{\frac{2}{3}}Pp_- \\ -\sqrt{\frac{2}{3}}Pp_z & 0 & 0 & 0 & \sqrt{\frac{1}{3}}Pp_- & 0 & 0 & 0 \\ Pp_- & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{1}{3}}Pp_z & 0 & 0 & -\Delta_0 & \sqrt{\frac{2}{3}}Pp_- & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}}Pp_+ & 0 & \sqrt{\frac{2}{3}}Pp_+ & E_0 & -\sqrt{\frac{2}{3}}Pk_z & Pp_- & \sqrt{\frac{1}{3}}Pp_z \\ -\sqrt{\frac{1}{3}}Pp_+ & 0 & 0 & 0 & -\sqrt{\frac{2}{3}}Pp_z & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}}Pp_+ & 0 & 0 & 0 \\ -\sqrt{\frac{1}{3}}Pp_+ & 0 & 0 & 0 & \sqrt{\frac{1}{3}}Pk_z & 0 & 0 & -\Delta_0 \end{pmatrix} \quad (2.14)$$

where P is the interband velocity operator matrix element $\langle jS|p_z/m_e|Z\rangle$ and it is often expressed in terms of the Kane energy $E_p = 2m_e P^2$. $p_{\pm} = \sqrt{1/2}(p_x \pm jp_y)$, E_0 and $-\Delta$ is the conduction band energy and split band energy at the zone center with zero set to be equal to the zone center energy of light hole and heavy hole band.

¹Light hole and Heavy hole bands are degenerate at $k=0$, and the corresponding eigenenergy is treated as 0.

2.4 Application of Kane model in heterostructures

2.5 The $\mathbf{k} \cdot \mathbf{p}$ model in this paper

In this work, we employ a modified first-order 8×8 Kane Hamiltonian to model the electronic band structure in semiconductor heterostructures. The original Kane model formulates the interaction between the conduction, light-hole, heavy-hole, and split-off bands near the Γ point within an 8-dimensional basis incorporating both the $\mathbf{k} \cdot \mathbf{p}$ interaction and spin-orbit coupling. We retain this original basis of total angular momentum eigenstates $|\mathbf{J}, \mathbf{M}_J\rangle$, given by equation 2.13, and with a similar Hamiltonian as the original Kane's model. A key extension in our formulation is the inclusion of an additional diagonal correction term D in the conduction band block of the Hamiltonian (H_{11}, H_{55}). The term D is defined as

$$D = \frac{1}{2m_e} p_z (1 + 2F) p_z + \frac{1}{m_e} p_+ (1 + 2F) p_- \quad (2.15)$$

, and it is derived via Löwdin's perturbative method, effectively captures the coupling between the conduction band and remote bands outside the 8-band basis, thereby improving the accuracy of the conduction band effective mass without the computational overhead of explicitly including higher-energy states in the Hamiltonian. The parameter F takes account of the remote band, therefore, the D represents the only 2^{nd} order effect in our model. Furthermore, to adapt the model for semiconductor heterostructures, we generalize the Hamiltonian by introducing spatially varying parameters $E_c(z)$, $E_v(z)$, $P(z)$, and $F(z)$, allowing the band-edge energies, interband momentum matrix elements, and spin-orbit splitting to vary along the growth direction. This enables the Hamiltonian to account

for band discontinuities, quantum confinement, and material inhomogeneities within the envelope function approximation. The resulting position-dependent Kane Hamiltonian describes the quantized subband structure and wavefunctions in quantum wells and superlattices while preserving the nonparabolicity, band mixing, and spin-orbit effects intrinsic to the multiband k·p formalism.

For completeness, we show the Hamiltonian here:

$$\begin{pmatrix} E_c + D & -\sqrt{\frac{2}{3}}Pp_z & Pp_+ & \sqrt{\frac{1}{3}}Pp_z & 0 & -\sqrt{\frac{1}{3}}Pp_- & 0 & -\sqrt{\frac{2}{3}}Pp_- \\ -\sqrt{\frac{2}{3}}Pp_z & E_l & 0 & 0 & \sqrt{\frac{1}{3}}Pp_- & 0 & 0 & 0 \\ Pp_- & 0 & E_h & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{1}{3}}Pp_z & 0 & 0 & E_s & \sqrt{\frac{2}{3}}Pp_- & 0 & 0 & 0 \\ 0 & \sqrt{\frac{1}{3}}Pp_+ & 0 & \sqrt{\frac{2}{3}}Pp_+ & E_c + D & -\sqrt{\frac{2}{3}}Pk_z & Pp_- & \sqrt{\frac{1}{3}}Pp_z \\ -\sqrt{\frac{1}{3}}Pp_+ & 0 & 0 & 0 & -\sqrt{\frac{2}{3}}Pp_z & E_l & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\frac{2}{3}}Pp_+ & 0 & E_h & 0 \\ -\sqrt{\frac{1}{3}}Pp_+ & 0 & 0 & 0 & \sqrt{\frac{1}{3}}Pk_z & 0 & 0 & E_s \end{pmatrix} \quad (2.16)$$

This Hamiltonian can be folded down to a 2x2 matrix

$$\begin{bmatrix} H_d & H_{nd} \\ H_{nd}^\dagger & H_d \end{bmatrix} \begin{bmatrix} \varphi_c \\ \varphi_{\bar{c}} \end{bmatrix} = E \begin{bmatrix} \varphi_c \\ \varphi_{\bar{c}} \end{bmatrix} \quad (2.17)$$

Here, we only explicitly show the expression for H_d since in our calculation, H_{nd} is neglected for computation efficiency consideration, since the φ_c computed does not differ significantly whether we consider the H_{nd} or not. What's more, the resulting splittings of

the momentum transfer by excluding H_{nd} remains within 1%. As a result, the continuity of the probability flux density at the heterointerfaces is not guaranteed[13].

$$H_d = \frac{1}{2m_e} p_z \left(1 + 2F + \frac{E_P}{3} \left(\frac{2}{E - E_l} + \frac{1}{E - E_s} \right) \right) p_z + \frac{\hbar^2 k^2}{2m_e} \left(1 + 2F + \frac{E_P}{6} \left(\frac{3}{E - E_h} + \frac{1}{E - E_l} + \frac{2}{E - E_s} \right) \right) + E_c. \quad (2.18)$$

with the corresponding effective mass defined as:

$$\frac{1}{m_{\parallel,\perp}(E, z)} = \frac{1}{m_e} \left[1 + 2F + \frac{E_P}{3} \left(\frac{2}{E - E_l} + \frac{1}{E - E_s} \right) \right], \quad (2.19)$$

One main result of using such 8 band $\mathbf{k} \cdot \mathbf{p}$ modeling is that there will be two spin groups with different phase relations within each group. [13]

2.6 Scattering Calculations

After deriving the wavefunctions and dispersion relations, we can move on to the calculation of scatterings. Since the $\mathbf{k} \cdot \mathbf{p}$ model results in two spin groups, there are two possible types of scattering, namely, the “same spin group” (SSG) scattering and the “different spin group” (DSG) scattering which preserves or flip the electron’s effective spin. The main scatterings considered in this thesis are LO phonon, impurity ions, interface roughness and alloy disorder scatterings in the context of an eight-band $\mathbf{k} \cdot \mathbf{p}$ model.²

²A more convenient form for LO, ION scattering can be found in [13]

2.6.1 LO Phonon Scattering

The expression for LO phonon Hamiltonian is:

$$H^{LO} = e\sqrt{\frac{E_{LO}P'}{2\Omega}} \sum_{\mathbf{Q}_{LO}} \frac{e^{-jQ_z\hat{z}}}{\epsilon\sqrt{Q_z^2 + Q^2}} e^{-\mathbf{Q}\cdot\boldsymbol{\rho}}, \quad (2.20)$$

, where the E_{LO} is the LO phonon energy. The factor P' is defined as $P' = (N_0 + \frac{1}{2} \mp \frac{1}{2})(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_s})$ with N_0 being the phonon occupation factor (i.e. the Bose-Einstein distribution at thermal equilibrium), and ϵ_∞ and ϵ_s are the material permittivities at high and low frequencies. Ω is the total volume. $\mathbf{Q}_{LO}$ is the phonon wavevector, and its magnitude of in-plane and z-direction components are denoted as Q, Q_z . The summation over $\mathbf{Q}_{LO}$ sums over all phonon wave vectors. ϵ is defined as $\epsilon = 1 + \frac{q_s^2}{Q^2 + Q_z^2}$ accounts for the electrostatic screening effect, and q_s is the inverse screening length. $\boldsymbol{\rho}$ is the position vector in real space. The scattering rate from initial state $|i, \mathbf{k}_i\rangle$ to subband f is calculated using the Fermi's Golden rule and is given by:

$$W_{if}^{LO}(k_i) = \frac{\pi e^2 E_{LO} P'}{(2\pi)^3 \hbar} \iint \frac{|\langle \psi_i | e^{-jQ_z\hat{z}} | \psi_f \rangle|^2}{Q^2 + Q_z^2} \delta(E_f - E_i \mp \hbar\omega) dQ_z d\mathbf{Q} \quad (2.21)$$

2.6.2 Impurity Scattering

The impurity scattering Hamiltonian is defined as:

$$H^{ION} = \frac{-e^2}{\Omega\epsilon_s} \sum_{\mathbf{q}_{ION}} \frac{e^{jq_z(\hat{z}-z_l)}}{q^2 + q_z^2 + q_s^2} e^{-\mathbf{q}\cdot\boldsymbol{\rho}}, \quad (2.22)$$

, where the Ω is the volume, ϵ_s is the material's low frequency permittivity, $\mathbf{q}_{ION} = (\mathbf{q}, q_z)$ is the impurity wavevector expressed in its in-plane and z-direction components, q_s is the inverse debye length, and ρ is the position vector.

Although on the first glance, this seems to have a different dimensionality compared to the LO Phonon Hamiltonian,

The expression for impurity scattering based on this Hamiltonian is:

$$W_{(if)}^{ION}(k_i) = \frac{1}{S\hbar} \left(\frac{e^2}{2\pi\epsilon_s} \right)^2 D_f(E_f^K) \int_0^{2\pi} \left| \int_{-\infty}^{+\infty} \frac{\langle \psi_i | e^{jq_z(\hat{z}-z_l)} | \psi_f \rangle}{\vec{q}^2 + q_s^2 + q_z^2} dq_z \right|^2 d\theta. \quad (2.23)$$

2.6.3 Interface roughness scattering

The expression for the interface roughness Hamiltonian is:

$$H^{\text{IFR}} = H(z_i + \Delta(\boldsymbol{\rho})) - H(z_i), \quad (2.24)$$

, where H is the 8-band Hamiltonian, z_i is the average longitudinal coordinate of the interface, $\Delta(\boldsymbol{\rho})$ is the roughness of the interface at position $\boldsymbol{\rho} = (x_i, y_i)$.

The expression for Interface roughness scattering is³:

$$W_{if}^{IFR}(k_i) = m_f \left(1 + \alpha_f^{\parallel} E_f^K \right) \frac{\pi \Lambda^2}{\hbar^3} \exp \left(-\frac{(k_f^2 + k_i^2) \Lambda^2}{4} \right) \sum_{\nu=0}^3 C^{(\nu)} I_{\nu} \left(\frac{\Lambda^2 k_f k_i}{2} \right), \quad (2.25)$$

, where m_f is the effective mass at the final state's band edge, $\alpha_f^{\parallel}$ is the in-plane non-

³For the exact expressions for $C^{(\nu)}$, one can find them in [13]

parabolicity parameter, E_f^K is the final state kinetic energy, Λ is the in-plane correlation length, Δ which is contained in the function C^ν is the mean roughness height, and $I_\nu(x) = \frac{1}{\pi} \int_0^\pi \cos(\theta) e^{x \cos(\theta)} d\theta$ is the modified Bessel function. For the special case of $k_i = 0$, we have[14]:

$$W_{\text{IFR}}(k_i = 0) = m_f \left(1 + \alpha_f^\parallel E_f^K\right) \pi \frac{\Lambda^2}{\hbar^3} \exp\left(-\frac{k_f^2 \Lambda^2}{4}\right) C^{(0)}, \quad (2.26)$$

, where the $C^{(0)}$ is defined as:

$$\begin{aligned} C^{(0)} \approx \Delta^2 \sum_{z_i} 4 \left[dV_c \phi_i^{(c)} \phi_f^{(c)} + dV_l \phi_i^{*(l)} \phi_f^{(l)} + dV_s \phi_i^{*(s)} \phi_f^{(s)} \right. \\ + \hbar^2 \frac{dF}{m_e} \partial_z \phi_i^{(c)} \partial_z \phi_f^{(c)} + j \hbar dP \left(\phi^{(v)} \partial_z \phi_i^{(c)} - \phi_i^{*(v)} \partial_z \phi_f^{(c)} \right) \\ \left. + \hbar dP \frac{k_f}{2\sqrt{2}} \phi_i^{(c)} \phi_f^{(h)} \right|_{z_i}^2 - dP^2 \left(\frac{\hbar k_f}{\sqrt{2}} \right)^2 \left(\phi_i^{(c)} \phi_f^{(i)} - \phi_i^{*(i)} \phi_f^{(c)} \right)^2 \Big|_{z_i} \Big], \end{aligned} \quad (2.27)$$

where we defined

$$\phi^{(v)} = -\sqrt{\frac{2}{3}} \phi^{(l)} + \sqrt{\frac{1}{3}} \phi^{(s)} \quad \text{and} \quad \phi^{(i)} = \sqrt{\frac{1}{3}} \phi^{(l)} + \sqrt{\frac{2}{3}} \phi^{(s)}.$$

In this approximation, the initial and final eigenfunctions ϕ_i and ϕ_f can be taken from the same or from different spin groups, and they are probed for each interface longitudinal position z_i . Obviously, by switching on or off the terms with dF and dP coefficients in equation 2.27, we can include or exclude the effect of remote band.

2.6.4 Alloy Disorder Scattering

The expression for alloy disorder Hamiltonian is:

$$H^{AD}(\mathbf{R}) = \sum_{\mathbf{R}_i \in R_A} (1-x)\delta V(\mathbf{R} - \mathbf{R}_i) - \sum_{\mathbf{R}_i \in R_B} x\delta V(\mathbf{R} - \mathbf{R}_i) \quad (2.28)$$

The equation for alloy disorder scattering rate calculation is then given by:

$$W_{if}^{AD}(k_i) = m_f \left(1 + \alpha_f^{\parallel} E_f^K\right) \frac{\Omega_0 x(1-x)V_{AD}^2}{\hbar^3} \sum_{s_i, s_f=E^+, E^-} \int \left| \phi_{i, k_i}^{(c, s_i)}(z) \phi_{f, k_f}^{(c, s_f)}(z) \right|^2 dz. \quad (2.29)$$

V_{AD} is defined as $\frac{1}{\Omega_0} \int_{\Omega_0} \delta V(\mathbf{r}) |u_{c0}|^2 d^3r$, where the $\delta V(r)$ is the difference between the two pure materials forming the alloy. For example, in GaAlAs, $\delta V(r) = V_{AlAs}(r) - V_{GaAs}(r)$. Therefore, V_{AD} is the spatial average of that difference, and the volume Ω_0 is the volume of one pure material. For example, in GaAs, a zinc-blende structure, each unit cell of the crystal contains four diatomic primitive cells, therefore, the Ω_0 for that is typically $\frac{a_0^3}{4}$. Note that, for AD scattering, we are only considering the conduction band. The effect of valence band is ignored, because if V_{AD} were defined in a similar manner for valence bands, the p-like orbital character, having a minimum at zero, would yield a V_{AD} much smaller than the conduction band value. Since conduction band states are s-like and have a greater amplitude at the lattice site, the valence band contribution is negligible in the final AD scattering rate.

2.7 Numerical Implementation

2.7.1 Finite Difference Method for eigenenergies and wavefunctions calculation

We follow a similar manner of derivation for the FDM method as in the Cooper's paper [40] with the effective mass replaced by 2.19. The analytical Schrodinger equation $H_d\varphi_c = E\varphi_c$ can be written as:

$$\left(-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \frac{1}{m_{\perp}(E, z)} \frac{\partial}{\partial z} + E_c - E + \frac{\hbar^2 k^2}{2m_{\parallel}(E, z)} \right) \varphi_c = 0, \quad (2.30)$$

and in the manner of difference approximation, we obtain:

$$\begin{aligned} & -\frac{\hbar^2}{2m_e\sigma_z^2} (\varphi_{c,z_{i+1}} - \varphi_{c,z_i}) \left[1 + 2F_{z_{i+1/2}} + \frac{E_{P,z_{i+1/2}}}{3} \left(\frac{2}{E - E_{l,z_{i+1/2}}} + \frac{1}{E - E_{s,z_{i+1/2}}} \right) \right] \\ & + \frac{\hbar^2}{2m_e\sigma_z^2} (\varphi_{c,z_i} - \varphi_{c,z_{i-1}}) \left[1 + 2F_{z_{i-1/2}} + \frac{E_{P,z_{i-1/2}}}{3} \left(\frac{2}{E - E_{l,z_{i-1/2}}} + \frac{1}{E - E_{s,z_{i-1/2}}} \right) \right] \\ & + \frac{\hbar^2 k^2}{2m_e} \left[1 + 2F_{z_i} + \frac{E_{P,z_i}}{3} \left(\frac{2}{E - E_{l,z_i}} + \frac{1}{E - E_{s,z_i}} \right) \right] \varphi_{c,z_i} + (E_{c,z_i} - E) \varphi_{c,z_i} = 0. \end{aligned} \quad (2.31)$$

By multiplying equation 2.31 by the denominators, and collect terms according to their

E's power, we are able to obtain a spare matrix representation:

$$\begin{bmatrix} 0 & I_{N_z} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{N_z} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_{N_z} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_{N_z} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{N_z} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I_{N_z} \\ A_0 & A_1 & A_2 & A_3 & A_4 & A_5 & A_6 \end{bmatrix} \begin{bmatrix} \varphi_c \\ E\varphi_c \\ E^2\varphi_c \\ E^3\varphi_c \\ E^4\varphi_c \\ E^5\varphi_c \\ E^6\varphi_c \end{bmatrix} = E \begin{bmatrix} \varphi_c \\ E\varphi_c \\ E^2\varphi_c \\ E^3\varphi_c \\ E^4\varphi_c \\ E^5\varphi_c \\ E^6\varphi_c \end{bmatrix}. \quad (2.32)$$

This sparse matrix can be efficiently solved using standard numerical libraries, and the resulting φ_c can then be used to reconstruct the wavefunctions of the other bands based on their known phase relationships.

2.7.2 Doping effects via Schrodinger-Poisson Self-consistent calculation

An initial evaluation of the band structure is ran at zero doping through the algorithm described in the last section. Then the more accurate band structure and charge distribution is calculated via an iterative self-consistent Schrödinger-Poisson solver by accurately accounting for doping-induced potential variations and charge redistribution. The total doping is gradually introduced in several small increments to improve numerical stability. At each doping step, the Poisson equation is solved using an initial estimation of the subband dispersions, and the Fermi level is updated based on the 2D carrier concentra-

tion. The median in-plane wavevector k is estimated to capture the representative in-plane occupation, and the corresponding Schrödinger equation is solved to obtain updated wavefunctions and subband energies. The electron density is then recalculated, and the process iterates until the electron density and potential converge self-consistently at this doping level. In the second stage, full in-plane k -resolved subband dispersions are calculated by solving the Schrödinger equation across the full k -space grid. Anti-crossings between subbands are tracked and relabeled at each k to maintain continuity of subband indices. A second Schrödinger-Poisson loop is then performed where the potential is updated using the full dispersion, with the median k -method employed to approximate the electron density at each iteration. Once this stage converges, a final self-consistent loop is performed in which the exact electron density is obtained by integrating the full wavefunctions across all occupied k -states, and the Poisson equation is updated accordingly. This final stage ensures that the electrostatic potential fully incorporates the actual quantum charge distribution derived from the complete in-plane subband structure.

Chapter 3

8 band model verification in InGaAs

To explore the result of using the 8 band Kane model described in the earlier chapter 2, we applied it on InGaAs/AlInAs QWs. From such simulation we can confirm that the measured electron lifetime can only be interpreted through a rigorous $\mathbf{k} \cdot \mathbf{p}$ approach that not only considers the hyperbolic subband dispersion but also band mixing k-dependence, which slows down all scattering mechanisms. This chapter includes content adapted from the author's previously published work [14], with permission.

3.1 Analysis of nondegenerate Pump Probe Experiment

3.1.1 Samples to analyze

Three distinct quantum well (QW) samples were analyzed to investigate subband population dynamics under various experimental conditions. The first sample, named QW-6, features a quantum well width of 6 nm. In this configuration, the system was excited using pump pulses that induced $1 \rightarrow 2$ intersubband transitions. Subsequent probe pulses monitored the carrier population in the lowest conduction subband across a range of in-plane wave vectors k , via interband transitions between the heavy-hole ground state and the conduction ground state. The second sample, referred to as QW-8, is an 8 nm wide QW structure. Here, the probe pulses investigate the population of the second conduction subband. In addition to these two, a third reference sample with a quantum well width of 10 nm was included. This sample was studied using differential absorption spectroscopy under continuous wave CO_2 laser pumping that excited $1 \rightarrow 2$ intersubband transitions, with probing focused on the conduction state. Due to the CW excitation scheme, this measurement carries a higher degree of uncertainty in determining the electron lifetime. In principle, we would want all the three samples being fabricated in the same lab and measured using the same techniques, however, there are no such three samples available in published literature. Here the QW-6 and QW-8 are from the same lab, while QW-10 is fabricated in a different molecular beam epitaxy (MBE) facility.

Table 3.1: Summary of InGaAs/AlInAs quantum well (QW) structures analyzed using $\mathbf{k} \cdot \mathbf{p}$ -based scattering theory.

Sample name	QW-6	QW-8	QW-10
Reference	[1]	[2]	[3]
Structure W(Å)/B(Å) $\times$ repeats	60/140 $\times$ 50	80/140 $\times$ 50	100/100 $\times$ 40
Doping type	δ -doping in center of barrier	δ -doping in center of barrier	3D doping in well
Doping concentration (cm^{-2})	1.5×10^{11}	5×10^{11}	6×10^{11}
$E_{21}(k=0)$ (meV)	251	191	129
$2 \rightarrow 1$ lifetime at 8 K (ps)	1.3	1.0	$\sim[0.6-1]$
Temperature (K)	8	8	[8-100]

3.1.2 Fitting of IFR and AD parameters (V_{AD} , Λ , Δ)

As discussed in previous sections, three material parameters relevant for modeling inter-subband dynamics are not well known: V_{AD} , Λ , Δ , they vary between different simulation tools and are highly debated. We define a combination of a specific value for each parameter that explain a set of experimental results as one 'triplet' and noted as ' T_n '. The subscript n represents the QW structure for which the triplet can be used in the simulation to fit the experimentally measured scattering times. For example, the triplet T_6 would fit the measured QW-6 scattering lifetime, and the triplet $T_{6,8}$ would simultaneously fit the experimental QW-6 and QW-8 lifetimes. Note that there can be more than one triplet that fit the two samples, therefore, we denote the set of triplets as $\{T_6\}$ for QW-6 and similarly $\{T_{6,8}\}$ for QW-6 and QW-8. In other words, multiple sets of these parameters might permit the superposition of four scattering processes to fit the experimental scattering lifetime, and the difference between each set lies in the relative weight of the AD and IFR scattering. As introduced previously, QW-6 and QW-8 are from the same lab, therefore, we first find a set of parameters $\{T_{6,8}\}$ fit both samples simultaneously to narrow down the possible values. Then use $\{T_{6,8}\}$ to simulate the total scattering time in the third sample,

QW-10. The subset of $\{T_{6,8}\}$ which agrees with the lifetimes reported in this “control” experiment in the same material system constitutes $\{T_{6,8,10}\}$.

In broad terms, Figure 3.1 represents the analysis method, which consists of simulating and fitting the experimental $2 \rightarrow 1$ intersubband lifetimes in the three samples (QW-6, 8, 10) using the same set of material parameters/triplets $\{T_{6,8,10}\} = \{(V_{AD}, \Delta, \Lambda)\}$, which are not well known yet. The colored subband dispersion is meant to show the $\mathbf{k}$ -dependent eigenstates, the color representing the “weight” of the c -band components defined as

$$w_c(k) = 2 \int |\varphi_{c,k}(z)|^2 dz. \quad (3.1)$$

This illustrates the importance of using the $\mathbf{k}$ -dependent eigenstates at the initial and final wavevector for the scattering calculation (the “M3” method).

The uncertainties of the reported Δ , Λ , and V_{AD} in $T_{6,8,10}$ depend on the experimental uncertainties of the pump-probe experiments. Since QW-6 and QW-8 samples did not report error bars, a Gaussian error function was assumed for the lifetime, assigning a standard deviation ς of 0.05 ps to the measured $2 \rightarrow 1$ intersubband transition lifetime. This assumption is reasonable, given that the probe laser pulse duration in the experiment is 0.1 ps. The probability density function for each sample is then defined by Eq. 3.2 where $\overline{\tau_{QW6}}=1.3$ ps and $\overline{\tau_{QW8}}=1.0$ ps (see last row in Table 3.1). When we simultaneously fit the data on QW-6 and QW-8 samples with a triplet $T_{6,8}$, the corresponding total probability density function is defined by Eq. 3.3. Later in the text, the probability density is reported without units, i.e. without the prefactor in front of the exponential because we assume the same standard deviation for both measurements in QW-6 and QW-8.

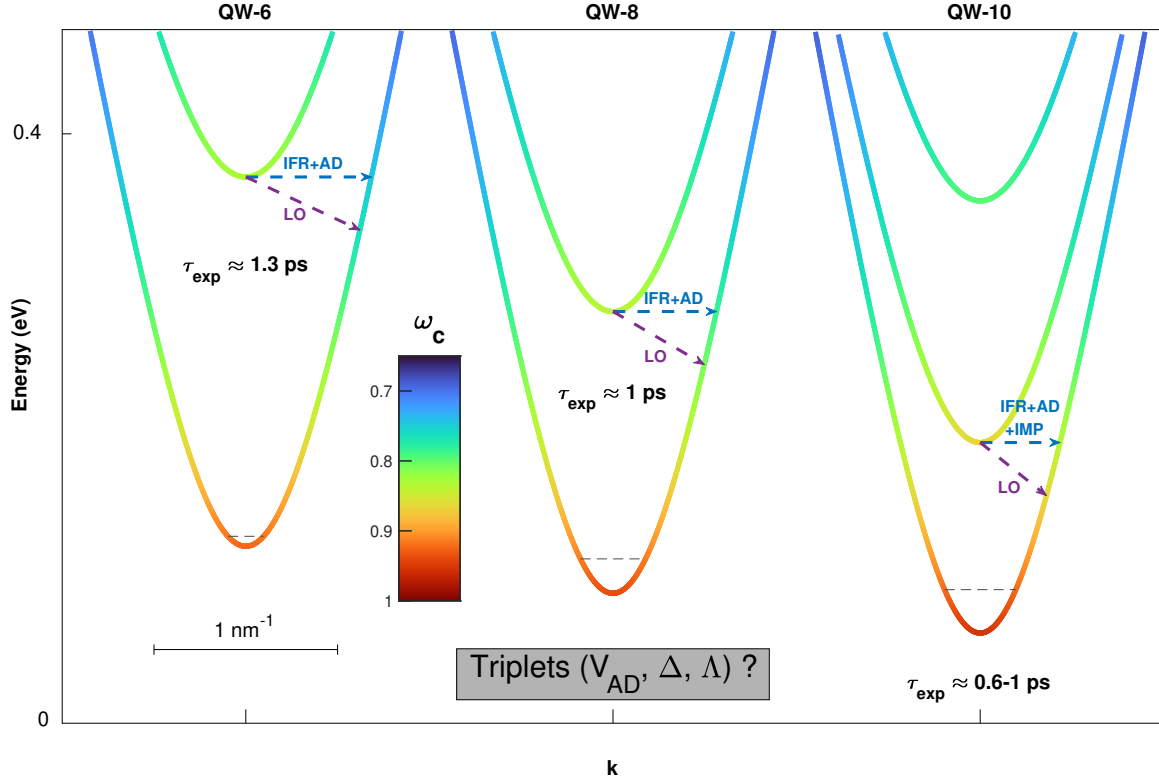


Figure 3.1: Conduction subband dispersion of QW-10, QW-8, and QW-6. The reference energy ($E=0$) corresponds to lowest energy in GaAs conduction band, including band bending caused by the Hartree potential. The color code on the subbands illustrates the “weight” of the c -band components versus k . The dashed arrows represent four different $2 \rightarrow 1$ intersubband scattering mechanisms that are considered in this analysis. The dashed line is the Fermi-energy. IMP (for impurity scattering) is not shown for QW-6 and QW-8 since those two samples are modulation-doped in the barrier, while QW-10 is uniformly doped in the well. The gray box asks if there could be triplets of material parameters $\{T_{6,8,10}\} = \{(V_{AD}, \Delta, \Lambda)\}$ that would account for the experimental intersubband lifetimes reported in [1], [2] and [3].

$$P_i(\tau_i^{\text{exp}}) = \frac{1}{\varsigma\sqrt{2\pi}} \exp\left(-\frac{(\tau_i^{\text{exp}} - \bar{\tau}_i)^2}{2\varsigma^2}\right), \text{ with } i = \text{QW6, 8.} \quad (3.2)$$

$$P_{\text{tot}}(\tau_{\text{QW6}}^{\text{exp}}, \tau_{\text{QW8}}^{\text{exp}}) = \frac{1}{2\pi\zeta^2} \exp\left(-\frac{(\tau_{\text{QW6}}^{\text{exp}} - \overline{\tau_{\text{QW6}}})^2 + (\tau_{\text{QW8}}^{\text{exp}} - \overline{\tau_{\text{QW8}}})^2}{2\zeta^2}\right) \quad (3.3)$$

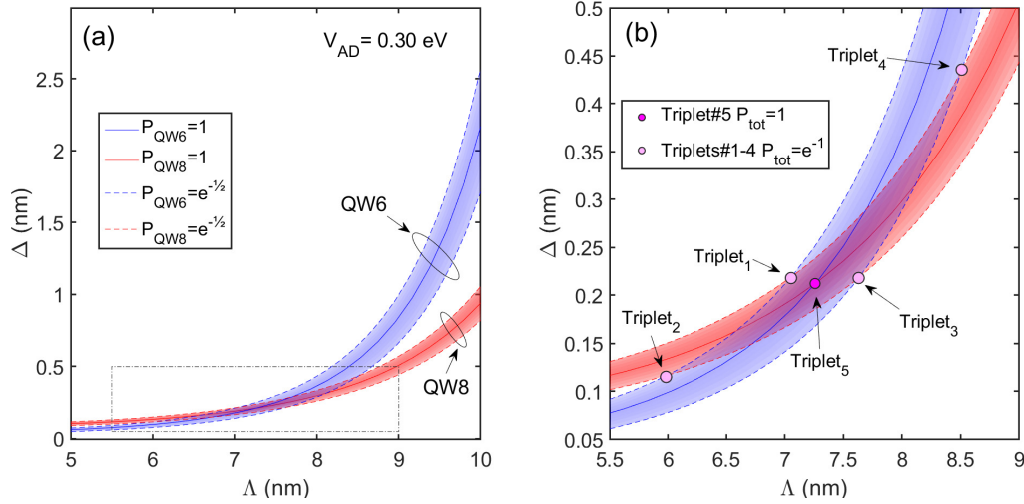


Figure 3.2: (a) Ensemble of IFR parameters fitting the experimental values of 2→1 intersubband lifetime in QW-6 and QW-8 samples. The color intensity of the graded colored ribbons corresponds to different P_{QW6} (blue) and P_{QW8} (red) values that are between 1 (vivid color) and $\exp\{-0.5\}$ (dimmed color). V_{AD} is fixed at 0.3 eV. When the two ribbons intersect, common Λ and Δ values can simultaneously fit QW-6 and QW-8 experimental lifetimes, hence the occurrence of $T_{6,8}$ triplets (V_{AD} , Δ , Λ). The solid lines represent the solutions with the highest probability ($P_{\text{QW6,8}} = 1$), and the dashed lines represent $P_{\text{QW6,8}} = \exp(-0.5)$. In (b), we show the zoomed-in section and label the five triplets that have $P_{\text{tot}} = \exp(-1)$ and $P_{\text{tot}} = 1$. The labeled triplets are: Triplet 1: $\tau_{\text{QW6}}^{\text{exp}} = 1.25$ ps, $\tau_{\text{QW8}}^{\text{exp}} = 0.95$ ps; Triplet 2: $\tau_{\text{QW6}}^{\text{exp}} = 1.25$ ps, $\tau_{\text{QW8}}^{\text{exp}} = 1.05$ ps; Triplet 3: $\tau_{\text{QW6}}^{\text{exp}} = 1.35$ ps, $\tau_{\text{QW8}}^{\text{exp}} = 1.05$ ps; Triplet 4: $\tau_{\text{QW6}}^{\text{exp}} = 1.35$ ps, $\tau_{\text{QW8}}^{\text{exp}} = 0.95$ ps; Triplet 5: $\tau_{\text{QW6}}^{\text{exp}} = 1.3$ ps, $\tau_{\text{QW8}}^{\text{exp}} = 1.0$ ps.

The details of the fitting procedure are as follows. We employ the most complete $\mathbf{k} \cdot \mathbf{p}$ based scattering models, i.e. M3 for LO phonon, impurity and AD scatterings, and M4 for IFR. First, LO phonon and impurity scattering are calculated and remain fixed for a given

quantum well structure. Based on this, we define a certain range of V_{AD} values to scan starting from zero. In each iteration, V_{AD} is thus fixed at a certain value while Δ , Λ are allowed to vary. To consider experimental uncertainty, the range of experimental intersub-band lifetime values is scanned from $\tau_{\text{QW6,8}}^{\text{exp}} = \overline{\tau_{\text{QW6,8}}} - 2.15\zeta$ to $\tau_{\text{QW6,8}}^{\text{exp}} = \overline{\tau_{\text{QW6,8}}} + 2.15\zeta$, corresponding to $0.1 \leq P_{\text{QW6,8}} \leq 1$. For each value of $W_{\text{QW6}}^{\text{exp}}$ and $W_{\text{QW8}}^{\text{exp}}$ we first find an ensemble of Δ , Λ parameters such that $W_{\text{LO}} + W_{\text{AD}} + W_{\text{IFR}} = W^{\text{exp}}$, as impurity scattering is negligible in QW-6,8. At this stage, all possible material parameters fitting the $2 \rightarrow 1$ relaxation time of each sample, QW-6 and QW-8, form the $\{T_6\}$ and $\{T_8\}$ triplet ensembles. An example is shown in Figure 3.2 for $V_{\text{AD}} = 0.3$ eV, where $\{T_6\}$ is represented by a bluish ribbon and $\{T_8\}$ by a reddish ribbon. If the two lines (blue for QW-6, red for QW-8) intersect at a specific (Δ, Λ) pair we obtain a solution, i.e. a $T_{6,8}$ triplet $(V_{\text{AD}}, \Delta, \Lambda)$ associated with the probability density $P_{\text{tot}} = P_{\text{QW6}}(\tau_{\text{QW6}}^{\text{exp}}) \times P_{\text{QW8}}(\tau_{\text{QW8}}^{\text{exp}})$. The fitting exercise is repeated for all V_{AD} in this range, as well as different $W_{\text{QW6}}^{\text{exp}}$ and $W_{\text{QW8}}^{\text{exp}}$ values. Figure 3.2(b) shows the intersection area of the two ribbons $\{T_6\}$ and $\{T_8\}$, which simply represents a large portion of triplets $\{T_{6,8}\}$ corresponding to $e^{-1} \leq P_{\text{tot}} \leq 1$. The same Figure 3.2(b) shows the graphic solution of four triplets with the same $P_{\text{tot}} = e^{-1}$ (see the dots named “Triplet₁₋₄”).

The shape of the ribbons in Figure 3.2 can be explained by using Eq. 3.4 because this equation accounts for the eight-band M4-IFR scattering model both qualitatively and even quantitatively.

$$W_{\text{IFR}}(k_i = 0) = \frac{\hbar}{\pi m_r} \Delta^2 \frac{4}{27} \frac{k_f^4}{\sqrt{1 + \frac{16}{3}(k_f r_{cv})^2}} f(\sigma), \quad (3.4)$$

where $f(\sigma) = \sigma^2 \exp(-\frac{1}{4}\sigma^2)$ is a bell-shaped function peaked at $\sigma = 2$ and σ is defined as $\sigma = k_f \Lambda$. m_r is the effective mass at the conduction band-edge, and r_{cv} is the interband dipole moment.

Knowing the function $f(\sigma)$ peaks at $\sigma = 2$ and rapidly decays for $\sigma > 2$ the ribbon's slope is stronger for QW-6 because in the chosen Λ range [5, 10 nm], $k_{f,QW6}\Lambda > k_{f,QW8}\Lambda > 2$. The range of $k_f \Lambda$ is [3.42, 6.84] for QW-6 and [2.83, 5.66] for QW-8. The square root terms of Eq. 3.4 due to the final density of states are similar in structures QW-6 and QW-8. To compare the two ribbons we can use $W_{\text{IFR}} \propto \Delta^2 k_f^4 f(\sigma)$. Therefore, the relative position between the ribbons can be explained by Eq. 3.5,

$$\frac{\Delta_{QW6}}{\Delta_{QW8}} \approx \sqrt{\frac{W_{QW6}^{\text{exp}} - W_{\text{LO},QW6} - W_{\text{AD},QW6}}{W_{QW8}^{\text{exp}} - W_{\text{LO},QW8} - W_{\text{AD},QW8}}} \times \sqrt{\frac{f(\sigma_{QW8})}{f(\sigma_{QW6})}} \times \left(\frac{k_{f,QW8}}{k_{f,QW6}}\right)^2. \quad (3.5)$$

This simplified expression explains the behavior of the ribbons (curvature and width) when V_{AD} changes. W_{AD} is about the same for QW-6 and QW-8. At $\Lambda=5$ nm, $f(\sigma)$ are comparable between the two samples $f(\sigma_{QW8}) \approx 1.7f(\sigma_{QW6})$ but at $\Lambda=10$ nm, $f(\sigma_{QW8}) \approx 30f(\sigma_{QW6})$. This explains why the Δ for QW-6 is much higher at large Λ for a fixed V_{AD} . When V_{AD} approaches its maximum value, the “room” left for IFR scattering is reduced on QW-6 sample, i.e. $W^{\text{exp}} - W_{\text{LO}} - W_{\text{AD}}$ decreases, while this term is still significant for QW-8. This is why the ribbon associated with QW-6 (the blue ribbon on Figure 3.2) gets flattened with V_{AD} increasing. Similarly, the width of the ribbon can be approached by the derivative of the simplified expression Eq. 3.6,

$$\delta\Delta = \frac{1}{2}\Delta \frac{\delta W^{\text{exp}}}{W^{\text{exp}} - W_{\text{LO}} - W_{\text{AD}}}. \quad (3.6)$$

3.1.3 Results and Discussions

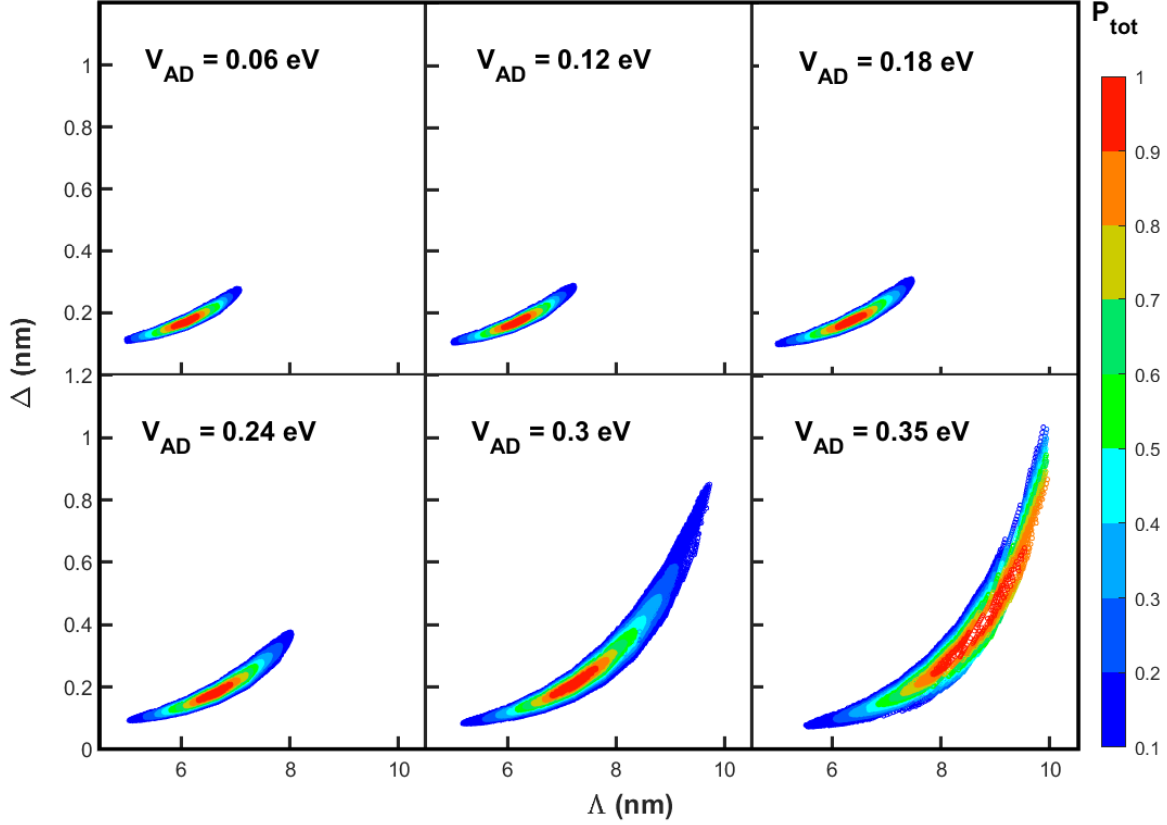


Figure 3.3: Triplets $\{T_{6,8}\}$ that fit both QW-6 and QW-8 simultaneously for six different V_{AD} values are plotted. Triplets $\{T_{6,8}\}$ are divided into different total probability bins according to the P_{tot} associated with them, and each probability bin is colored with different colors.

Figure 3.3 shows the $\{T_{6,8}\}$ triplets with P_{tot} ranging from 0.1 to 1 for six V_{AD} values for QW-6 and QW-8. We selected the range of by taking into account the experimental central scattering rate (i.e., at $P_{\text{QW6,8}} = 1$) and assuming $\Delta = 0$. The maximum V_{AD} is

0.377 eV on QW-6, and with QW-8, we obtain 0.504 eV. Since the overlap of [0,0.377] eV and [0,0.504] eV gives [0,0.377] eV, only the triplets with V_{AD} within that range are relevant. Figure 3.3 shows a general shift to larger Λ values as V_{AD} increases. This occurs because, for both samples, $k_f\Lambda > 2$. To compensate for the increasing W_{AD} , W_{IFR} needs to decrease, which implies that $k_f\Lambda$ should be larger (resulting in a smaller $f(\sigma)$). For example, we take two triplets with $P_{tot} = 1$, ($V_{AD}=0.3$ eV, $\Delta = 0.212$ nm, $\Lambda=7.262$ nm) and ($V_{AD}=0.24$ eV, $\Delta = 0.183$ nm, $\Lambda=6.658$ nm), their corresponding products $\Delta\Lambda$ are 1.539 nm^2 and 1.212 nm^2 . The products are a bit higher than 1.01 nm^2 derived in Ref. Tsujino2005 and 0.973 nm^2 derived in Ref. Wittmann2008, which are based on the measurement of the linewidth of intersubband spontaneous emission.

Our analysis suggests lower V_{AD} values than those commonly used in the QCL community [41, 42, 43, 44, 45]. However, our relatively low V_{AD} value aligns with those derived from more recent fits of mobility measurements in $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$ quantum wells [46, 47]. Regarding the indium dependence of V_{AD} , which is notably minimal for $x > 0.5$, we refer to Ferry and Phillips’s electronegativity theory [48, 49], as summarized in Van Vechten’s paper [50]. On the other hand, we acknowledge that our AD model is highly simplified, introducing more uncertainty in the proposed V_{AD} values. To better visualize the suggested triplets, Figure 3.4 displays solutions with total probability density greater than 90%.

We consent it is optimistic to rely on $P_{tot} > 90\%$ solutions only, given the resolution of pump-probe experiments. Using the triplets $\{T_{6,8}\}$ of Figure 3.4, the scattering rates for QW-10 and QW-4.5 are simulated and finally plotted vs. V_{AD} in Figure 3.5. For the scope of the discussion, QW-4.5 is a “theoretical structure” similar to QW-6, with 4.5 nm InGaAs

QWs, centered doped in the barrier but not measured with pump-probe techniques. QW-10 with uniform doping in the well shows a significant contribution from impurity scattering, and therefore the relative weight of IFR+AD scatterings remains small. The accuracy of the pump-probe experiment is insufficient to select the triplet at $V_{AD}=0.25$, or 0.3 eV for instance. The same problem is also predicted with QW-4.5 even though this sample is tuned at high intersubband energy $E_{21} = 282$ meV at $k=0$. The two structures in Figure 3.5 have a rather weak dependence on V_{AD} . This is understandable because AD and IFR scatterings are not very well decoupled processes, since their form factors are similar. Using a prosaic language, we could say AD and IFR scattering “walk hand-in-hand”, which undermines the chance to decrease the volume of $\{T_{i,j,k}\}$ triplets by using three samples (i, j, k) whose $2 \rightarrow 1$ intersubband dynamic was measured by optical pump-probe setups. Since the problem is to choose material parameters among many triplets, it looks almost unavoidable to have an independent measurement of the interfaces via the characterization techniques such as ultra-high vacuum scanning tunneling microscopy (UHV-STM) [51, 52] or atom probe tomography (APT) [53, 54] or electron tomography based on high-angle annular dark-field scanning transmission electron microscopy (HAADF-TEM) [55, 56]. Alternatively, other mobility measurements could confirm the low AD potential derived in this study. If the objective of the fitting exercise were to propose an exact triplet to the scientific community, this work could be considered inconclusive, due to the inherent resolution of the pump-probe experiment and the fact that AD and IFR form factors are not sufficiently independent of each other. Nevertheless, if low V_{AD} values can be confirmed independently, this study has narrowed the range of IFR parameters. In broad terms AD and IFR scatterings are rather correlated, therefore, the choice of the exact triplet should

not have a large impact on the total intersubband dynamic in a QCL. Albeit QW-10 is grown in another lab and its $2 \rightarrow 1$ intersubband relaxation is measured by a different technique, we note the simulated lifetime falls inside the experimental error bar for most of V_{AD} values, which tends to support the $\mathbf{k} \cdot \mathbf{p}$ -based scattering theory.

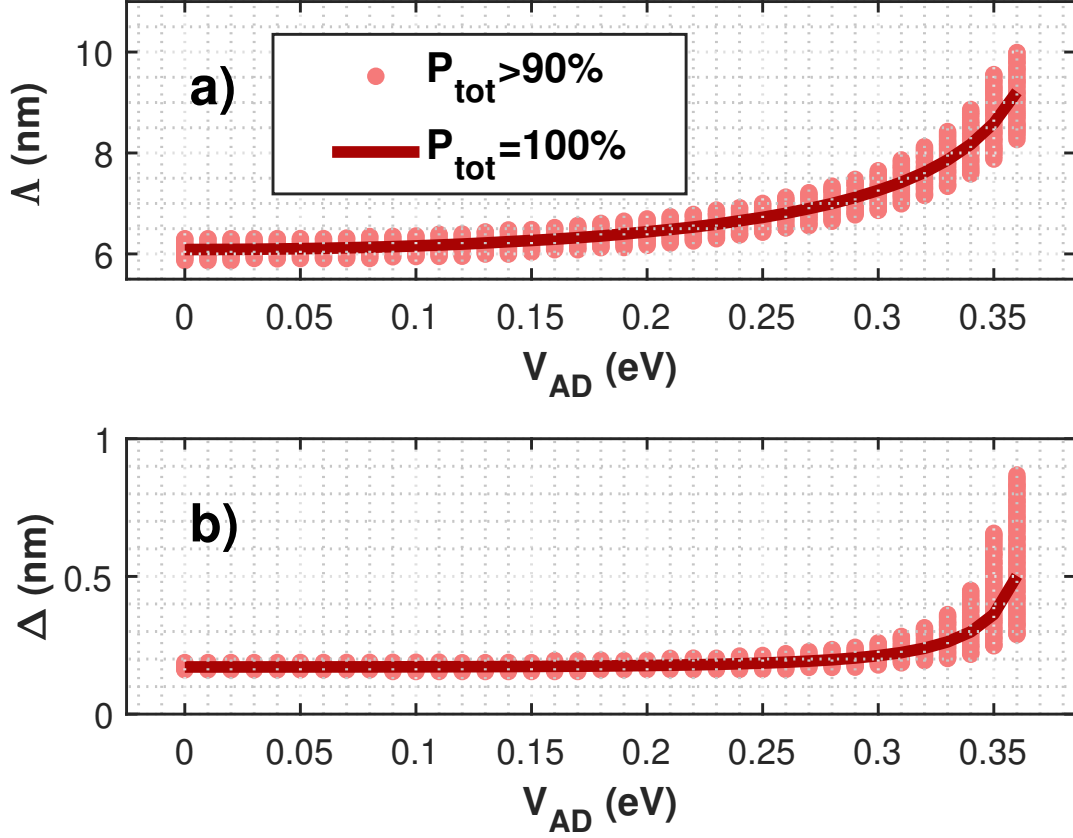


Figure 3.4: a). Λ versus V_{AD} for triplets $\{T_{6,8}\}$ corresponding to $P_{\text{tot}} > 0.9$. b). Δ versus V_{AD} for triplets $\{T_{6,8}\}$ corresponding to $P_{\text{tot}} > 0.9$.

The fitted triplets are utilized to simulate the three quantum well structures, QW-6, QW-8, and QW-10, using various methods M1 to M4. Those methods are defined in Table 3.2. Specifically, we focus on a particular triplet with $P_{\text{tot}} = 1$, which is $T_{6,8} = (V_{AD}=0.3 \text{ eV}, \Delta=0.212 \text{ nm}, \Lambda=7.262 \text{ nm})$. As Figure 3.6 shows, for M1, the one-band $\mathbf{k} \cdot \mathbf{p}$ model, the calculated 2-1 LO Phonon intersubband scattering rate alone has already exceeded the experimental total scattering rate. This leaves no room to include other scattering

Table 3.2: Band-mixing model simplifications

Method	Description
M1	Uses only ϕ_c normalized to unity, $\mathbf{k}=0$ eigenstates.
M2	Includes l and s valence bands, $\mathbf{k}=0$ eigenstates.
M3	Includes all 8 bands, consider $\mathbf{k}$ -dependence of eigenstates.
M4-IFR	Includes 8 bands, $\mathbf{k}$ -dependent eigenstates, and interfacial perturbations to F and P for IFR.

mechanisms into the model. For M2, there is also very little room for other scattering mechanisms. Only when M3 or M4 is used, LO phonon, impurity, AD, and IFR can be included to match the measured scattering rate. We claim that the one-band model is not enough for modeling intersubband devices in this wavelength range. In addition, the ratio W_{M4}/W_{M1} for QW-6, QW-8, and QW-10 are 0.602, 0.642 and 0.714, respectively, demonstrating a consistent increase in the band mixing effect at shorter wavelengths. In QW-10, impurity scattering contributes to the total intersubband lifetime. In reality this contribution could be smaller in case of dopant segregation, which would bring the total M4 scattering closer to the central experimental value of 1.28 ps^{-1} . Simulations versus temperature were run on QW-10 up to 100 K; as expected the total lifetime decreases slightly with temperature but always stays within the experimental error bar reported in Ref. [3]. However, the same paper shows a slight lifetime *increase* versus temperature not explained yet (from $\sim 0.78 \text{ ps}$ at 8 K to $\sim 0.82 \text{ ps}$ at 100 K).

3.1.4 Conclusion

This study revisits pump-probe experiments that measure the intersubband electron dynamics in InGaAs/AlInAs quantum wells using an eight-band $k \cdot p$ model. With this model,

we examine the importance of $\mathbf{k}$ -dependent band-mixing in interpreting/fitting these experiments. The eight-band model takes into account the conduction band, heavy-hole band, light-hole band, and split-off band following Kane’s formalism. The results highlight the remarkable capabilities of the refined $\mathbf{k} \cdot \mathbf{p}$ model, which is capable of including LO phonon, alloy disorder, interface roughness, and impurity ion scattering. The commonly used simple one-band models (M1) inadequately represent the intersubband dynamics. Indeed, the one-band model gives faster rates than eight-band model, leaving no room for the inclusion of several critical scattering processes to account for the pump-probe experimental results. We underscore this analysis was based on experimental data obtained from MBE materials grown in the mid-nineties, and therefore, it would be of great interest to repeat this exercise with newer state-of-the-art structures.

Through a systematic fitting of three pump-probe experimental lifetimes, this work suggests a range of IFR and AD parameters (V_{AD}, Δ, Λ). Due to the inherent experimental inaccuracy, as well as the correlated nature of IFR and AD scattering parameters, it is challenging to further narrow down those parameters by this naive fitting method. Notably, the suggested alloy disorder potential (V_{AD}) values are lower than commonly assumed in the QCL community, aligning more closely with recent mobility-based studies. Such challenges invoke the need for complementary characterization techniques such as ultra-high vacuum scanning tunneling microscopy or electron tomography to refine these parameters further. It would also be appropriate to perform a similar analysis by taking into account the graded interfaces caused by In surface segregation (provided that they are characterized first by atom probe or electron tomography) and by using a more general IFR scattering theory[53, 57].

Despite this, our work demonstrates the validity and necessity of including the $k \cdot p$ theory to model intersubband dynamics. It paves the way for refined QCL designs that would take into account band mixing's $\mathbf{k}$ -dependence, in conjunction with more realistic IFR and AD materials parameters. However, additional material characterizations remain necessary to confirm the proposed Δ , Λ and V_{AD} values.

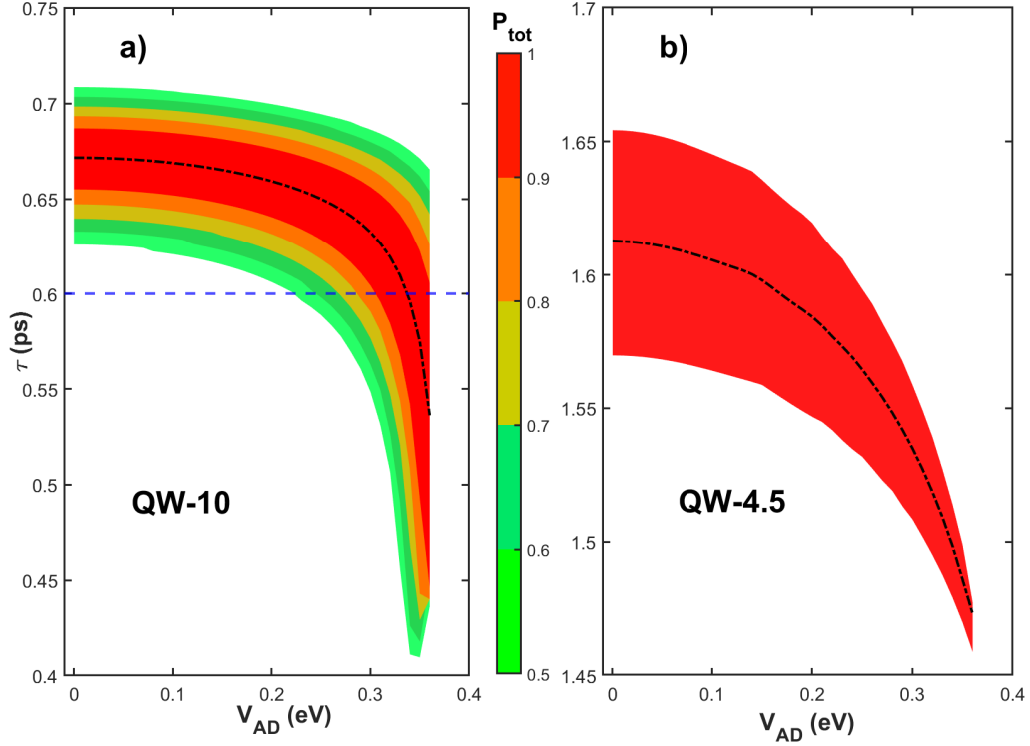


Figure 3.5: Simulated scattering time for QW-10 and QW-4.5 at 8 K with the triplets $\{T_{6,8}\}$ from QW-6 and QW-8. a). The results using $\{T_{6,8}\}$ triplets corresponding to five different probability bins are plotted. The blue dashed line is the experimental lower bound for QW-10. The upper bound should occur at 1 ps, and it is not shown in the plot. The black dash-dotted line corresponds to triplets with $P_{tot} = 1$. b). The result for QW-4.5 is shown with the ≥ 0.9 bin's triplets only.

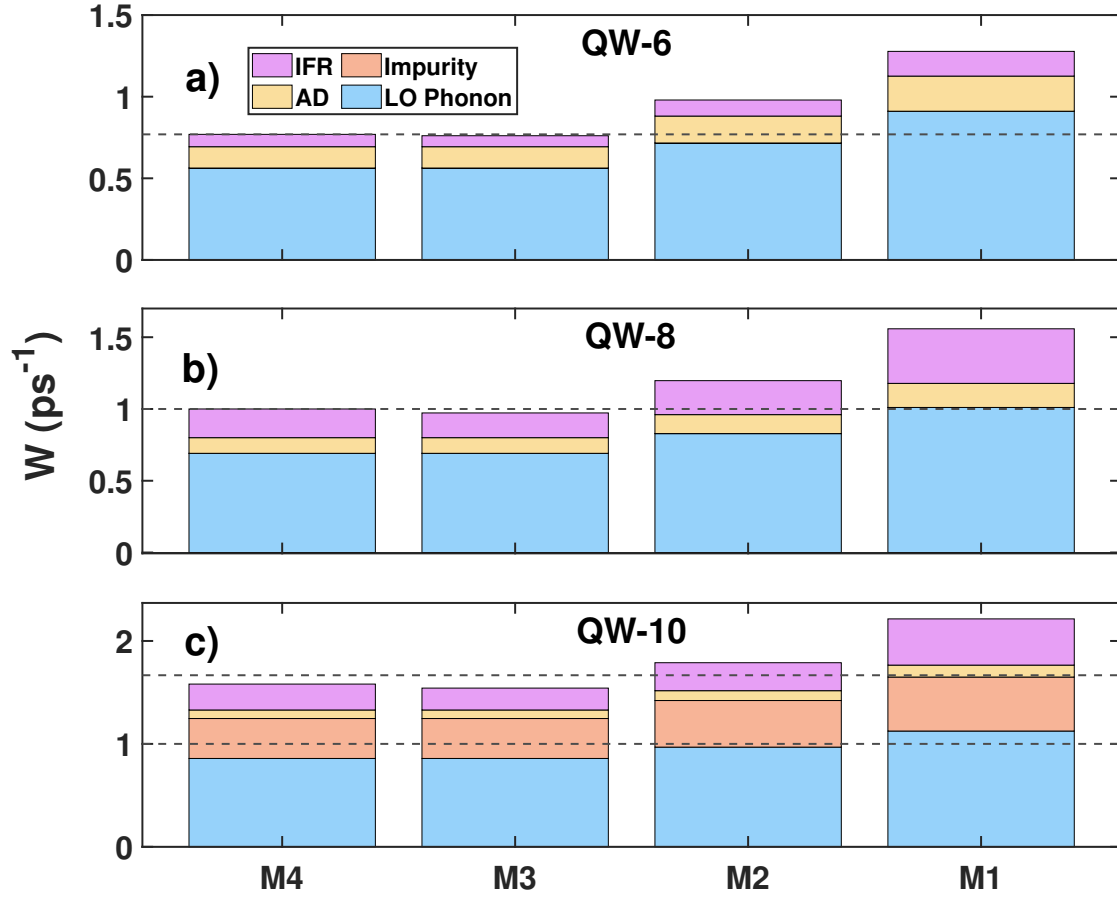


Figure 3.6: Different portions of the total scattering rate are shown for all the three samples using the triplet $T_{6,8}=(V_{\text{AD}}=0.3 \text{ eV}, \Delta = 0.212 \text{ nm}, \Lambda = 7.262 \text{ nm})$ at 8 K. The dashed lines are the experimental scattering rate. a) The dash line represents $W_{\text{QW6}}^{\text{exp}} = 0.77 \text{ ps}^{-1}$. b) The dash line represents $W_{\text{QW6}}^{\text{exp}} = 1 \text{ ps}^{-1}$. c) The dash lines represent $W_{\text{QW10}}^{\text{exp,L}} = 1 \text{ ps}^{-1}$ and $W_{\text{QW10}}^{\text{exp,H}} = 1.67 \text{ ps}^{-1}$.

Chapter 4

k-dependent confinement effects

As stated in previous chapters, understanding how electrons scatter within a quantum cascade laser (QCL) is crucial for accurately modeling their performance. One important yet often overlooked factor is how the shape and position of wavefunctions change with momentum, which directly affects scattering rates and device efficiency. According to Fermi's Golden Rule, the scattering rate is governed by the form factor $\langle \psi_i | H_{scat} | \psi_f \rangle$, which is clearly influenced by the overlap between the initial $|\psi_i\rangle$ and final $|\psi_f\rangle$ wavefunctions. Since the wavefunction shape varies with different k-values, the overlap between two states will also change when the k-dependence of the wavefunctions is taken into account. This effect is called the “k-dependent confinement effects”. For instance, at $k=0$, the wavefunction in a heterostructure may extend over several wells with a large spatial spreading, however, as k increase, the wavefunction will be more concentrated or localized in one well. In this chapter, we will demonstrate such k-dependent confinement effects by simulating two InAs/AlSb QCLs. Both QCLs use a diagonal transition scheme. Table 4.1 shows the

details of those QCLs. QCL-B operates at room temperature with an emission wavelength of $12.9 \mu m$, while QCL-A operates at a cryogenic temperature of 80 K and emits at a wavelength of $19.7 \mu m$. The methodology is pretty straight forward, and is demonstrated in Fig. 4.1. The QCL structure is input into the $k \cdot p$ model, which calculates the corresponding eigenenergies and eigenstates. These results are then used to analyze how the overlap between the upper and lower lasing states evolves as the lower lasing state moves away from the zone center¹. The quantity “static dipole”, defined in the later section, is used to quantify the spatial separation between the two wavefunctions.

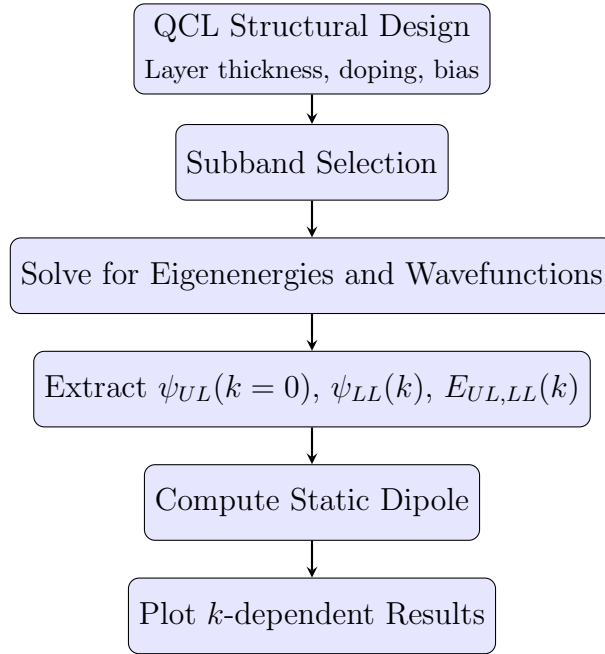


Figure 4.1: Workflow for evaluating k -dependent confinement effects using the 8-band $\mathbf{k} \cdot \mathbf{p}$ model.

¹For clarity, the Upper/Lower Lasing Level (ULL/LLL) or State (ULS/LLS) refers to the quantized energy levels between which electrons emit photons. In our study, the upper state is kept fixed at zero in-plane momentum ($k = 0$), while the lower state is varied with different k values.

Table 4.1: Summary of QCLs with Relevant Parameters

QCL Name	Temp(K)	$\lambda(\mu\text{m})$	Structure	ULL-LLL (Label)	Bias (kV/cm)	Doping (cm^{-3})
QCL-B[25]	300	12.9	[21 43 3 63 2.4 66 3 63 3.2 57 6.3 60 9.4 61 10.6 56 11.6 53 12.6 52 12.6 49]	11 – 10	–32	5×10^{16}
QCL-A[58]	80	19.7	[20 73 3 127 2 108 2 100 5 <u>98</u> 8 100]	6 – 5	–20	1×10^{17}

4.1 Dispersion And Wavefunctions

The two structures defined in Table. 4.1 are simulated using the 8-band k.p model developed in chapter 2. This model can compute wavefunctions for different subbands at all relevant positions and at various k-values, as well as, the dispersion relation for each subbands. The resulted E-k relation is shown for both QCLs in Fig. 4.2. The Upper and Lower Lasing states are determined by the energy difference between them at $k=0$. For example, in Fig. 4.2.b), the energy difference between the dotted ULS and the dashed LLS equals to 0.0926 eV, which corresponds to a wavelength of $13.3 \mu\text{m}$ and it's close to the experimentally measured value $12.9 \mu\text{m}$. One important feature observed in the dispersion diagram of Fig.4.2.a) is the presence of an anticrossing around $k \approx 5 \times 10^8 \text{m}^{-1}$. This anticrossing, arising from strong coupling between adjacent subbands, complicates the calculation of scattering rates because transitions may involve a superposition of multiple

subbands. A possible strategy to handle this complexity is to sum up the scattering contribution from both the ULL and the adjacent subband (ULL+1) into the LLL. A similar anticrossing also happens for QW-B at around $k = 9.5 \times 10^8 m^{-1}$. However, in the present work, we intentionally fix the initial ULS at $k = 0$, as intraband scattering is generally rapid enough to maintain electrons near the bottom of the subband. This simplification allows us to avoid the complications and focus solely on how the final-state wavefunction evolves with increasing k .

The probability density of each subband in real space at $k = 0$ is shown in Fig. 4.3, and Fig. 4.4 for QW-B, and QW-A correspondingly. In the probability density plot, the bottom of each curve corresponding to the subband energy at $k=0$. The height of each curve represents the magnitude of probability density at that location. For example, in Fig.4.3, the dotted curve representing the ULL exhibits a peak in the first well, followed by progressively smaller amplitudes in the second, third, and fourth wells. This spatial profile indicates that electrons in the ULL are primarily localized in the first well, with limited penetration into adjacent wells. In contrast, the dashed curve representing the LLL in QCL-A shows comparable amplitudes in the third and fourth wells, a moderate peak in the fifth well, and a smaller tail extending into the sixth well. This broader spatial distribution suggests that the LLL wavefunction is more delocalized, spreading over a larger portion of the heterostructure. In a similar way, in Fig.4.4, the ULL is also localized in the first well, while the LLL is spread in space. Typically, scatterings between all possible subband pairs need to be considered for a most accurate modeling, but that would be very computationally expensive. In QCL modeling, a clean n-level system is usually assumed so that only the scatterings among those related n number of levels are computed. Here, since

the purpose is only to demonstrate the k-dependent confinement effect, in other words, how the change of k value in one subband alters the scattering rate, only the ULL and the LLL is considered. The ULL state is fixed at $k=0$, and the LLL state is varied at different k values.

4.2 Overlap and static dipole

Fig 4.5 and 4.6 show the probability density for the ULL and the LLL. As k increases, the probability distribution of the LLL becomes more localized in the wider well and shifts closer to the peak of the ULL wavefunction. The blue curve represents the probability distribution of the LLL at $k \approx 0$. As discussed in the previous section, the LLL at this point is broadly distributed across several quantum wells in both QCL structures. However, as the wavevector k increases, a noticeable change occurs: the peak probability in the second quantum well nearly doubles for QCL-A and triples for QCL-B. Simultaneously, the amplitudes in the surrounding wells diminish significantly. This shift indicates that the LLL becomes increasingly localized in the second well with rising k, demonstrating the k-dependent confinement effect. The enhanced localization alters the spatial overlap with the ULL and directly impacts the form factor $\langle \psi_i(k_i) | H_{scat} | \psi_f(k_f) \rangle$ governing scatterings.

To quantify the spatial separation between the two wavefunctions, we introduce the static dipole defined as $\delta_{UL}(k) = |\langle z_{uls,k=0} \rangle - \langle z_{lls,k} \rangle|$ which measures the absolute difference between the expectation values of position for the ULS (at $k=0$) and the LLS (at varying k values). A smaller dipole implies more spatial overlap, which often corresponds to stronger scattering or emission rates. The static dipole for different final state kinetic energies are

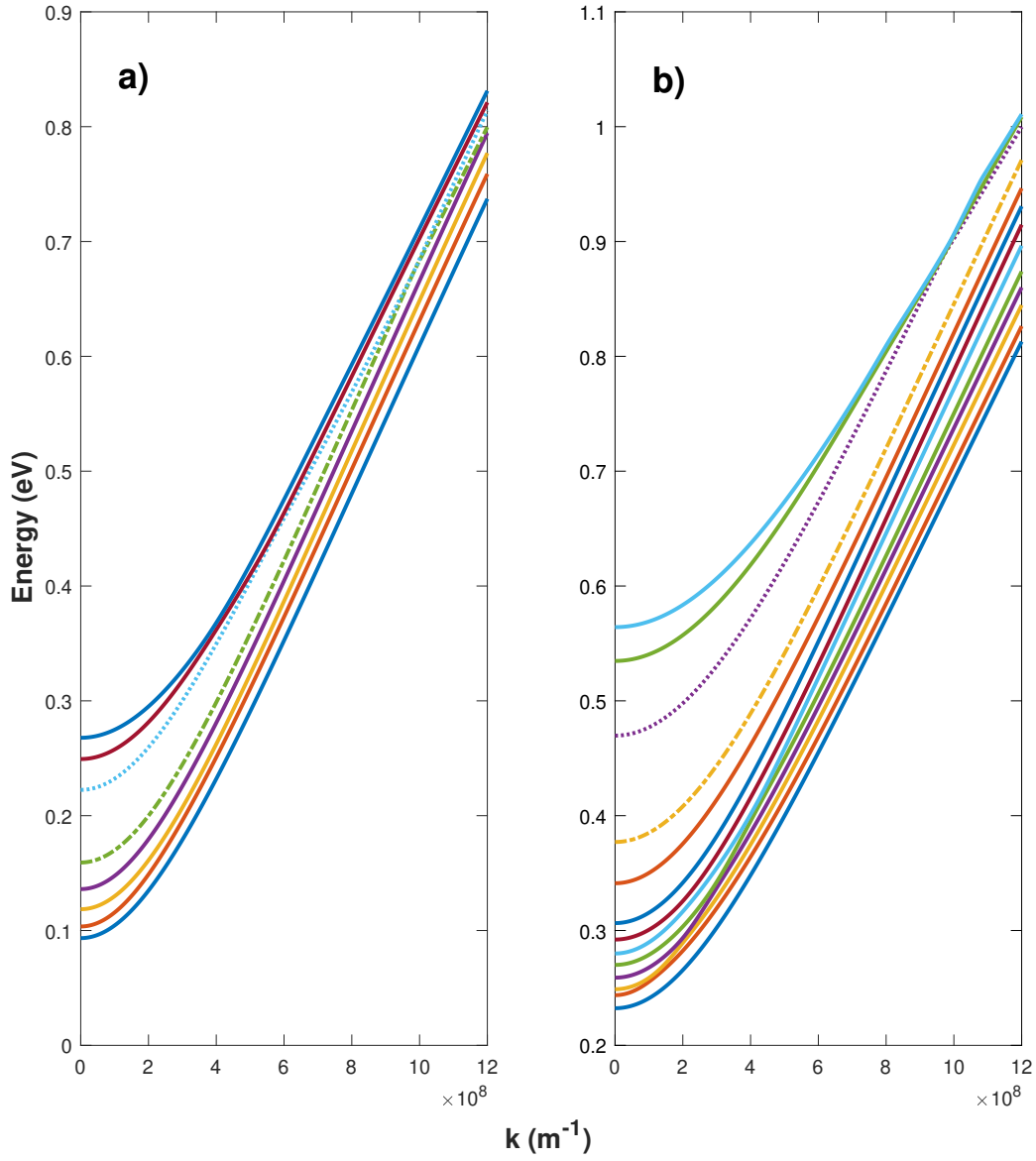


Figure 4.2: This figure shows the energy-wavevector ($E-k$) dispersion relations for each quantum well. The dotted line denotes the upper lasing state, while the dash-dot line indicates the lower lasing state. a) for QW-A, and b) for QW-B.

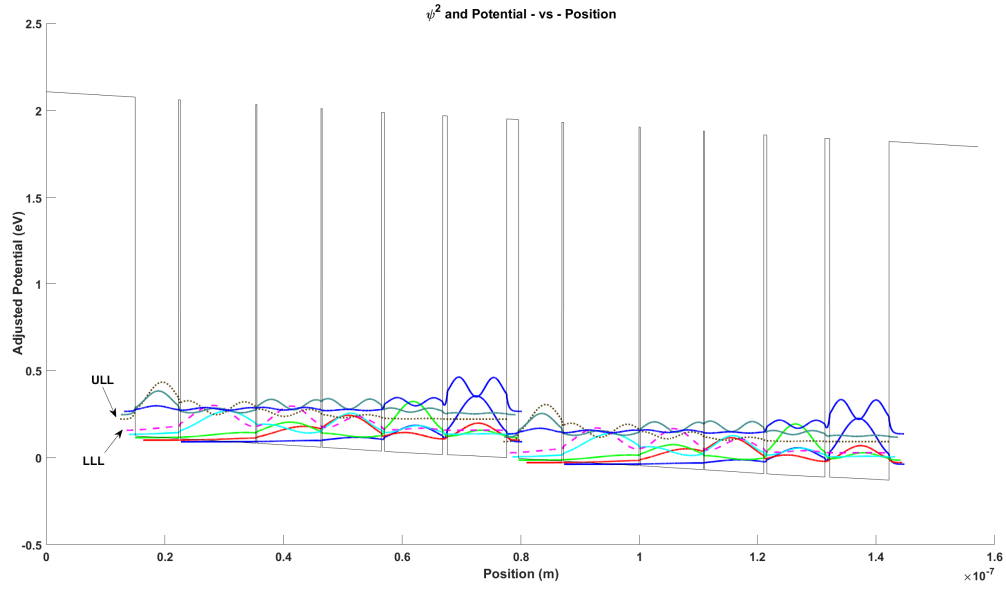


Figure 4.3: The wavefunctions/eigenstates @ $k=0$ for QW-A over two periods. The Upper Lasing Level (ULL) and the Lower Lasing Level (LLL) are denoted by a dotted line and a dashed line correspondingly.

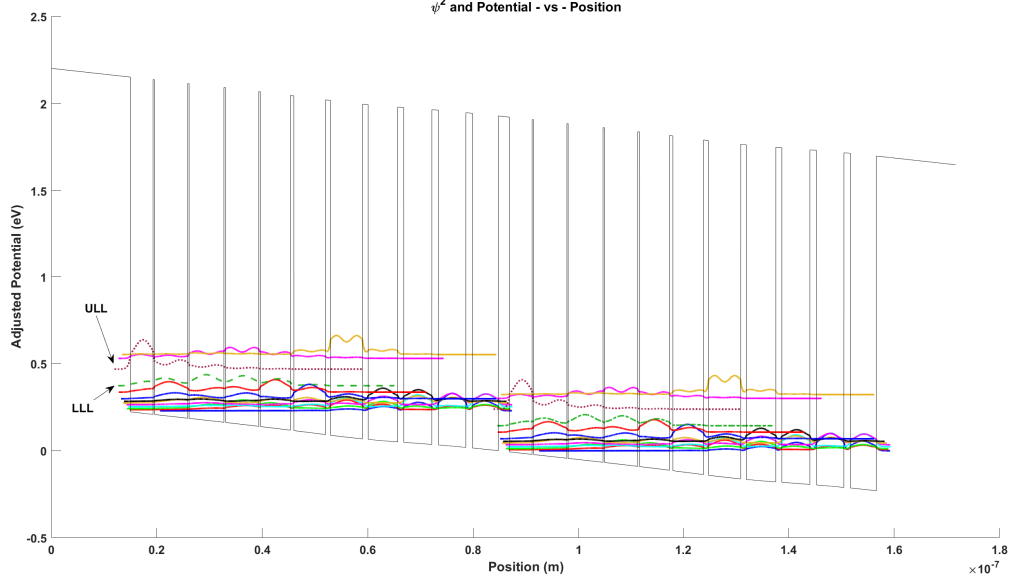


Figure 4.4: The wavefunctions/eigenstates @ $k=0$, for QW-B over two periods.

shown in Fig. 4.7.

When the final state kinetic energy is 0, the static dipole for QW-A and QW-B are 9.19 and 10.36 nm correspondingly. As the kinetic energy increases to $E_{if}(k=0)$, their static dipoles reduce to 6.64 and 7.59 nm. The reason we care about the kinetic energy $E_{if}(k=0)$ is that for elastic scattering, like impurity, interface roughness and alloy disorder scattering, the LLS will have exactly this energy after scattering, and for LO Phonon scattering, the LLS will have the kinetic energy at $E_{if}(k=0) - E_{LO}$.

Therefore, in certain diagonal QCL designs, the scattering transition can become significantly less diagonal than the corresponding optical transition when the LLS is treated as in a k -dependent manner. As a result, the spatial overlap relevant to scattering may increase compared to that predicted by conventional three-band models, where all wave-

functions are evaluated only at $k = 0$. This can lead to enhanced scattering rates despite the nominally diagonal nature of the design. Such an enhanced scattering rate between the ULS and LLS is generally undesirable, as these two subbands are intended to facilitate radiative optical transitions. Excessive nonradiative scattering between them can undermine the population inversion, which is essential for sustained lasing. Consequently, this degrades the overall performance of the QCL.

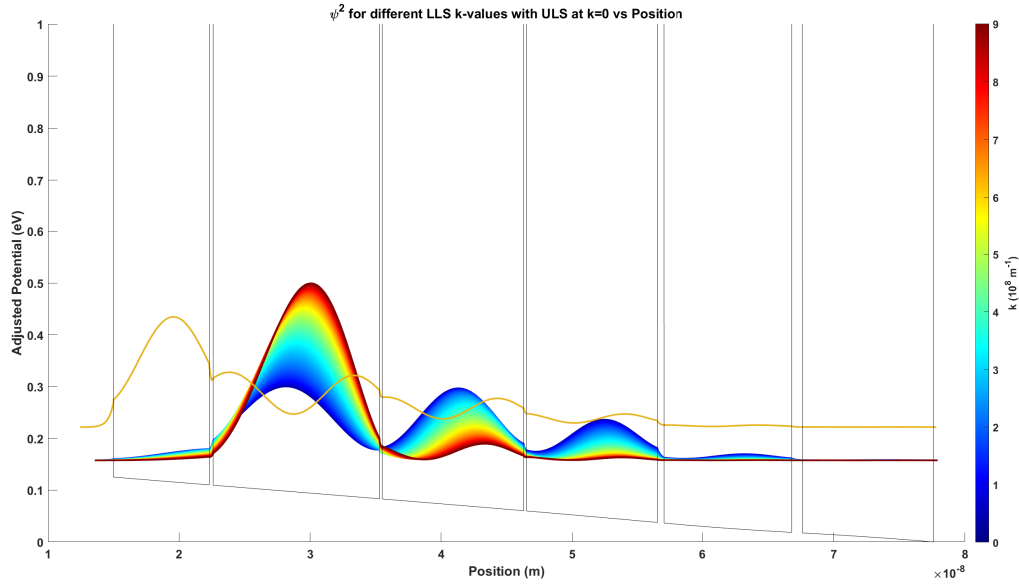


Figure 4.5: The ULS probability function is fixed at $k=0$, while the LLS probability function is varied from 0 to $9 \times 10^8 \text{ m}^{-1}$ for QCL-A

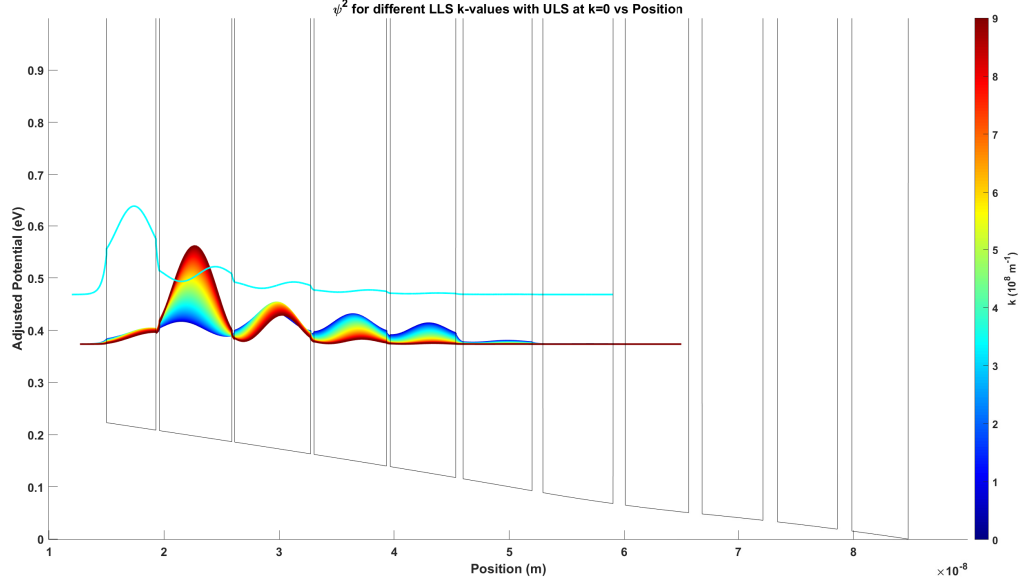


Figure 4.6: similar to Fig. 4.5, but for QCL-B

4.3 Conclusion

This chapter presented a quantitative analysis of the k -dependent confinement effect in two InAs-based QCL structures, emphasizing how wavefunction overlap, as well as, scattering form factor vary with the final-state kinetic energy or equivalently the final state wavevector. We demonstrated that as the wavevector k of the LLS increases, its wavefunction becomes increasingly localized in specific wells, shifting closer to the ULS's spatial profile. This enhanced overlap was captured through the static dipole metric, which showed a significant reduction (by around 27%) over the range of relevant final-state energies.

These results underscore the importance of incorporating k -dependent wavefunctions into scattering rate calculations. Models that neglect this effect, such as the most com-

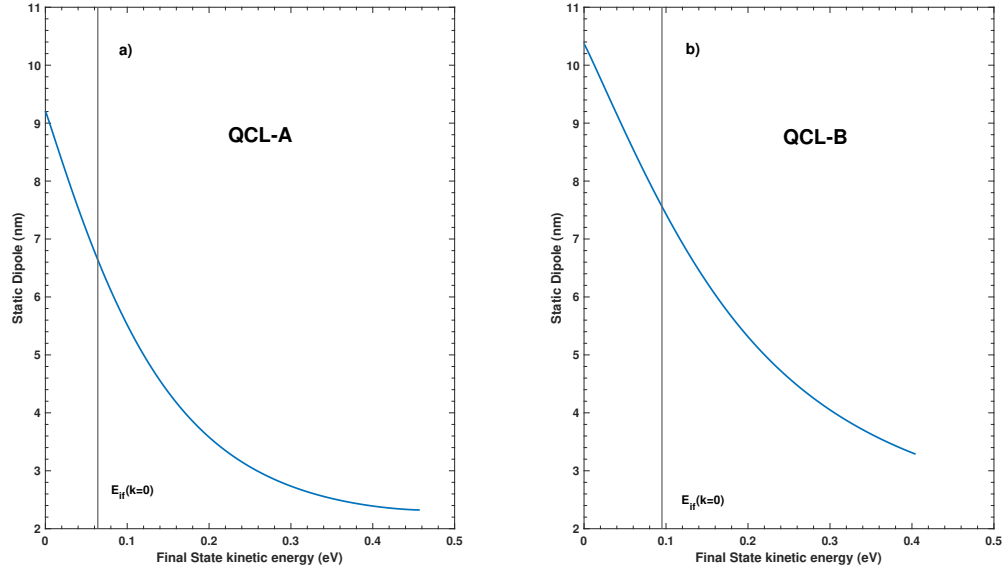


Figure 4.7: The static dipole for a) QCL-A, and b) QCL-B at different final state kinetic energies. The vertical line labeled as $E_{if}(k = 0)$ corresponds to the energy equals to the energy difference between the ULS and the LLS at $k=0$

monly used three-band model which evaluates all wavefunctions at $k = 0$, can significantly underestimate the spatial overlap between subbands. This can lead to an underestimation of nonradiative scattering rates, ultimately resulting in inaccurate predictions of device performance. From a device design perspective, this analysis suggests that even diagonal QCL structures can experience non-negligible nonradiative losses due to wavefunction reshaping at finite momentum. As such, design strategies must consider not only the spatial probability distribution of subbands at $k = 0$, but also how the final-state wavefunctions evolve for different kinetic energies. In future work, the full scattering rates can be calculated with k -dependent wavefunctions, and plugging those results into the rate equations would give a full transportation model for QCL structures. Such a model would provide a more accurate physical insight into the internal carrier, such as the nonradiative losses between ULS and LLS. Ultimately, this would offer valuable guidance for optimizign the QCL designs.

Chapter 5

Conclusion

5.1 Summary of Contributions

This thesis presents a k -dependent 8-band $k \cdot p$ model to simulate scattering rates in semiconductor quantum wells (QWs) and quantum cascade lasers (QCLs). Two major contributions are made:

First, the model was validated through fitting scattering rates, computed using the 8-band $k \cdot p$ method, to experimental pump-probe data obtained from InGaAs/AlInAs quantum wells. By incorporating nonparabolic dispersion, multiband wavefunction mixing, and k -dependent eigenstates, the proposed framework accurately reproduces experimental lifetimes and identifies a constrained range for interface roughness (IFR) and alloy disorder (AD) parameters ($V_{AD} = 0.3$ eV, $\Delta = 0.212$ nm, $\Lambda = 7.262$ nm). This fitting demonstrates that a simplified one-band or three-band model can significantly overestimate scattering

rates by up to 66%, especially in narrow-gap systems, due to their inability to capture valence band contributions and wavefunction reshaping. The three pump probe experiments alone are not sufficient to give the exact IFR and AD parameters, further narrow down of these parameters ranges might be achieved by additional surface information derived from UHV-STM.

Second, the model was applied to investigate k -dependent confinement effects in InAs/AlSb-based QCLs. Through simulation of two QCL structures, it was shown that the LLS's wavefunction becomes increasingly localized with rising k wavevectors. This spatial reshaping alters the overlap with the ULS and significantly impacts the form factor in Fermi's Golden Rule. The concept of the static dipole, introduced to quantify this spatial separation, revealed a 27–28% reduction in dipole length over the relevant kinetic energy range. These results establish that even nominally diagonal designs can experience increased nonradiative scattering when k -dependent effects are considered, which may degrade population inversion and device performance.

From those two main contributions, we conclude one most important claim: Conventional scattering models that evaluate wavefunctions only at $k = 0$ may lead to substantial under- or overestimation of scattering rates in QCLs, particularly in diagonal designs. Therefore, multiband coupling and k -dependent wavefunctions should be rigorously incorporated in simulation of QCLs, as these effects substantially influence scattering rates and carrier transport.

5.2 Limitations

While the 8-band $k \cdot p$ model presented here captures key physics of band mixing and momentum dependence, it still relies on several simplifications:

- The remote band effects are only considered for conduction band.
- The ULS is fixed at $k = 0$, which assumes a rapid thermalization process - an assumption that may not hold at elevated temperatures or in THz QCLs with reduced LO phonon efficiency.
- The simulation time increases significantly due to the necessity to compute wave-functions at all relevant k values.

5.3 Future Work

From the results of this thesis, several directions can be pursued to further advance the modeling of QCLs:

- Integrate this framework into rate equation or density matrix electron transport model with additional electron temperature calculations to provide a self-consistent for even more accurate scattering rate calculations. This can eventually lead to the simulation of a real QCL structure.

- A 4-band model can actually be achieved by a change of basis from this 8-band model. The reduction in the basis functions can lead to a significant reduction in the simulation time. This is essential when the structures get complicated.
- Furthermore, once a complete and accurate electron transport model is established for QCL structures, machine learning or genetic algorithms could be employed to automatically generate or optimize device designs. Utilizing such methods could significantly accelerate the discovery of novel QCL structures, particularly for challenging regimes such as room-temperature Terahertz QCLs. This integration of physical simulation model with intelligent optimization would represent a powerful tool for next-generation QCL design.

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