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Article

Optical Absorption and Raman Scattering in ZnO/Mg_xZn_{1-x}O Quantum Wells Under Non-Resonant Laser Effect

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Abstract: The influence of a non-resonant intense laser field on the optical absorption and Raman scattering processes in ZnO/Mg_{0.2}Zn_{0.8}O quantum wells is theoretically investigated. It is shown that the dressing field significantly modifies the confinement potential and reshapes the electronic wave functions, leading to tunable shifts in intersubband transition energies and changes in the dipole matrix elements. These laser-induced effects produce notable variations in the absorption spectrum and strongly modulate the Raman differential cross section and Raman gain. Under the application of the non-resonant laser field, the Raman gain is enhanced by almost a factor of four, whereas off-resonant pumping results in much weaker but still field-dependent responses. The results demonstrate that intense laser fields provide an effective tool to dynamically control the optical and Raman properties of ZnO-based quantum well structures.

Keywords: ZnO/MgZnO quantum wells; non-resonant intense laser; linear optical absorption; Raman differential cross section; Raman gain

1. Introduction

Semiconductor quantum wells (QWs) are of high importance in the investigation of nanophotonics and optoelectronic devices due to their quantized electron states and highly tunable optical properties. Among the multiple QW systems that can be found in the literature, the ZnO-based heterostructures have been receiving great attention in the last decades due to their prominent optical properties in the blue-ultraviolet (UV) region of the spectrum [1–3], wide bandgap semiconductivity, advantages in fabrication, native defects [4], large exciton binding energy [5], and other thermal, optical, and electronic properties.

The intrinsic features of the ZnO-based systems make them suitable for many applications, such as terahertz (THz) technologies [6], quantum Hall effect (QHE) devices [7], High Electron Mobility Transistors (HEMTs) [8], heterojunction photodiodes (HPDs) [9], light-emitting diodes (LEDs) [10], etc. Particularly, in the development of ZnO-based heterostructures, Mg_xZn_{1-x}O alloys have been widely investigated and employed for optoelectronic devices thanks to their tunable and higher bandgap structure [11], which goes from 3.37 eV in ZnO to 7.8 eV in MgO; furthermore, the Mg doping does not cause great lattice distortion and produces further adjustments in the carrier concentration and decreases leakage current [12].

Among ZnO-based heterostructures, ZnO/Mg_xZn_{1-x}O QWs are of typical interest due to their confinement properties, which allow an increase in the concentration of localized 2D electron gas [13] and enhanced electron mobility (up to 20 cm²/V) [14]. These structures are well produced via multiple growth methods, such as molecular beam epitaxy, thermal vapor deposition, and pulsed

laser deposition [15–17], and they present a very important feature: ZnO/MgZn_xO_{1-x} QWs exhibit significant spontaneous and piezoelectric polarization along the c-axis [18–20], which strongly modifies the confinement potential due to these built-in electric fields.

Beyond material composition, optoelectronic and additional properties of heterostructures are strongly influenced by the geometry and dimensions of the confinement potential. This feature has been largely demonstrated in the study of quantum dots (QDs) systems, particularly in GaAs-based nanostructures, which serve as a well-founded benchmark for low-dimensional confinement effects. For example, Gil-Corrales et al. in 2025 [21] studied the effects of different configurations (size and shape) on confined non-interacting particles that influence the thermodynamic features of GaAs QDs, resulting in practical properties for optical and Raman devices. Furthermore, in 2026 [22] again in three-dimensional systems, has been analyzed the additional effect of external electric fields and nonextensive statistics in QDs. These works tell that the confinement engineering, including geometrical design or external perturbations are central in controlling quantum states in semiconductor heterostructures.

Due to this, there has been a vast and in-depth study of the effects of external laser fields in multiple systems based on heterostructures. Specifically, the study of non-resonant intense laser fields (ILFs) has become a major focus of recent research in condensed matter, mainly due to the tailoring of optical and electronic properties resulting from the tunability of the confinement potential along the laser polarization direction [23]. For example, Wang et al. in 2021 [24] reported the tailoring effect of external fields via a terahertz ILF on the shallow-donor-related photoionization cross section in GaAs bulk semiconductors. Donado et al. in 2025 [25] reported the particular effect of combining an external electric field and an ILF on the electronic properties of a truncated cone quantum dot, in which the quantum confinement can be controlled by the dressing parameter α_0 . Additionally, Dagua et al. in 2025 [26] reported the effects of ILF on the probability of electronic transmission in QW AlGaAs/GaAs resonant tunneling diodes based on the Pösch-Teller potential.

All of the effects on the quantum confinement properties of a heterostructure will have a noticeable impact on optical absorption, which plays an important role in the characterization of these systems. In the case of the ZnO-based heterostructures, Tang et al. in 2025 [27] investigated the generation of double peaks in the inter-band and inter-subband optical absorption in Mg_xZn_{1-x}O/Al_yGa_{1-y}N core-shell nanowires, depending on the core radius and different crystal phases, while Gu et al. in 2022 [28] reported the shift of the peak positions in the total optical absorption coefficient in MgZnO/ZnO double QWs due to the variation of external electric and magnetic fields. As additional literature, Andrzejewski et al. in 2021 [29] carried out the experimental measurement and theoretical comparison of the photoluminescent spectra of multiple grown asymmetric QWs with different widths and internal electric fields, considering single particle transitions and localized excitonic contributions to the photoluminescence depending on temperature. Lastly, Atic et al. in 2024 [30] showed numerically how the Mg concentration and doping density affect the inter-subband absorption peak and tunneling current in different configurations of multiple ZnO/MgZnO QWs and resonant-tunneling structures in order to mimic the active regions of a quantum cascade laser.

Additionally, there are modifications to the light-matter interactions as a result of quantum confinement and changes in the electronic density of the system. One of these phenomena is the inelastic scattering of incident photons due to their interaction with electrons, which produces emitted radiation at shifted frequencies depending on the type of transition occurring in the system (Stokes/anti-Stokes) [31,32]. These processes are known as Raman processes, which can be effectively characterized using the differential cross section (DCS) of electron Raman scattering. The DCS quantifies the probability per solid angle and per unit frequency interval that an incident photon will be scattered, serving to determine the subband structure and electron density distribution in heterostructures. For example, Mojab-Abpardeh et al. in 2018 [33] performed the theoretical calculation of the DCS in the strained ZnO/MgZnO double QWs, successfully determining the impact of the system dimensions on the presence of new peaks in the cross-section. More recently, Betancourt-Riera et al. in 2025 [34] re-

ported the effect of an external electric field on the Raman emission spectra for intersubband transitions in semiconductor nanowires.

Another important feature that characterizes the Raman process is the gain coefficient, which measures how a heterostructure amplifies an optical probe via stimulated Raman scattering when pumped by a strong optical field. Since the Raman gain is directly related to the imaginary part of the third-order susceptibility, it is prone to being affected by nonlinearities in the system. For example, Tiutiunnyk et al. in 2020 [35] studied the effect of asymmetric step-like InGaAs/GaAs QWs on the enhancement of the Raman gain, especially with the inclusion of conduction-band non-parabolicity that permits a direct comparison of deviations with the most traditional parabolic models. Furthermore, Elamathi et al. in 2020 [36] calculated the impact of hydrostatic pressure and geometric confinement on the nonlinear optical properties of a confined exciton in InP/ZnS core/shell quantum dots, including the shift of the Raman intensity toward a higher Raman gain due to applied hydrostatic pressure.

Although Raman scattering in nanomaterials and nanostructures has been extensively investigated, systematic and recent studies of the Raman differential cross section and Raman gain in ZnO/MgZnO quantum well systems remain scarce and difficult to find. However, it is still possible to find some related works on Raman scattering in ZnO-based structures. Among the mentioned works, Tran et al. in 2022 [37] reported the successful fabrication of surface-enhanced Raman spectroscopy substrates based on ZnO/Au nanorods, which offer great signal enhancement and can be further amplified under UV excitation. Additionally, Samriti et al. in 2024 [38] also reported the excellent performance of ZnO/Ag nanohybrid substrates for surface-enhanced Raman scattering applications.

In the present work, we investigated the modification of confinement properties, linear optical absorption, Raman DCS and Raman gain in a ZnO/Mg_{0.2}Zn_{0.8}O QW with internal electric fields under the influence of a non-resonant ILF. Through the theoretical framework of the envelope function approximation, considering fixed temperature, piezoelectric and spontaneous polarization, and dressing-dependent carrier densities, we examine how the dressing parameter alters the confined energy levels, dipole matrix elements, optical absorption coefficient, and lastly the Raman DCS and Raman gain. These results highlight the potential for optical field tailoring of QW properties, paving the way for the development of tunable photonic devices of ZnO-based systems.

This paper is organized as follows: In Section 2, we schematize the system and the theory, including the main equations used for the dressed potential, optical absorption, DCS, and Raman gain. In Section 3, our main results are presented and discussed. Finally, in Section 4, we present our concluding remarks.

2. Theory

2.1. ZnO/Mg_xZn_{1-x}O Heterostructure

The system consists of an asymmetric Quantum Well, where the well (ZnO) and the barriers (Mg_xZn_{1-x}O) have dimensions of $L_w = 6$ nm and $L_b = 8$ nm, respectively, the concentration of Mg has been fixed at $x = 0.2$, see Figure 1. Following [39], the total potential U consists of two parts: the band offset and the built-in electric fields resulting from piezoelectric and spontaneous polarization, and is given by:

$$U(z) = \begin{cases} eF_b z + \Delta E_c, & 0 < z < L_b, \\ eF_w z + e(F_b - F_w)L_b, & L_b < z < L_b + L_w, \\ eF_b z + e(F_w - F_b)L_w + \Delta E_c, & L_b + L_w < z < L, \end{cases} \quad (1)$$

where z is the growth direction of the structure, F_w, F_b are the values of the built-in electric fields inside the well and the barrier, respectively, ΔE_c is the conduction band discontinuity and L is the total length of the system. These internal electric fields are calculated by

$$F_w = \frac{2L_b P_{\text{tot}}}{2\epsilon_b L_b + \epsilon_w L_w}, \quad F_b = -F_w \frac{L_w}{2L_b}, \quad (2)$$

where P_{tot} is the total contribution from piezoelectric and spontaneous polarization in the whole system, and $\epsilon_{w,b}$ are the dielectric constants for the well and barrier, respectively. Additionally, the band discontinuity can be defined as a percentage of the difference between the bandgaps in the junction, for this case

$$\Delta E_c = Q \left(E_{g,\text{Mg}_x\text{Zn}_{1-x}\text{O}} - E_{g,\text{ZnO}} \right), \tag{3}$$

where $Q = 0.75$ is the $\text{Mg}_x\text{Zn}_{1-x}\text{O}/\text{ZnO}$ band offset, which is a typical value according to the literature (citar papers). The multiple parameters used for the heterostructure, including the dependencies on the Mg concentration, internal electric fields and band discontinuity values, can be found in Table 1. The corresponding values of ZnO can be obtained by putting $x = 0$.

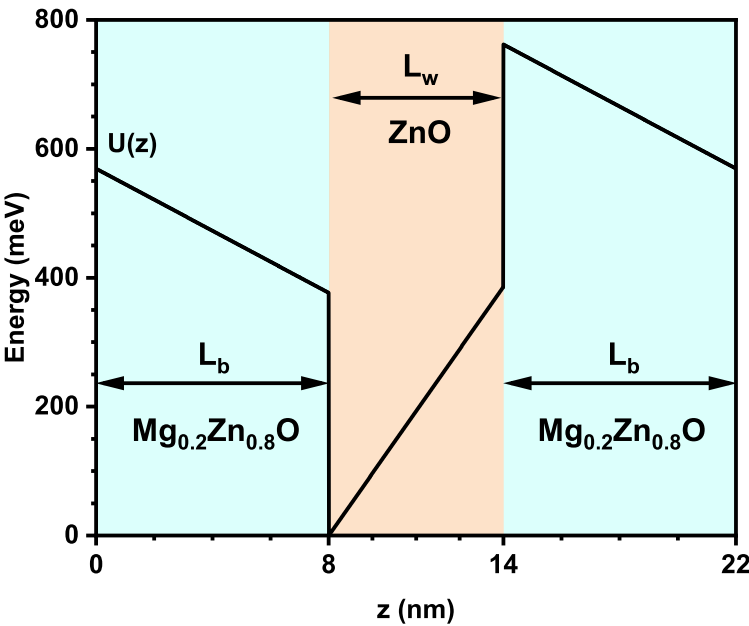


Figure 1. Potential profile $U(z)$ represented in the $\text{ZnO}/\text{Mg}_{0.2}\text{Zn}_{0.8}\text{O}$ QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm.

Table 1. Parameters used for the $\text{ZnO}/\text{Mg}_x\text{Zn}_{1-x}\text{O}$ QW calculation.

Parameter (units)	$\text{Mg}_x\text{Zn}_{1-x}\text{O}$
Vacuum electron mass m_0 (kg)	9.11×10^{-31}
Reduced Planck constant $\hbar$ (eV s)	6.58×10^{-16}
Boltzmann constant k_B (eV/K)	8.62×10^{-5}
Vacuum permittivity ϵ_0 (F/m)	8.85×10^{-12}
System temperature T (K)	300
Well internal electric field F_w (MV/cm)	-0.24
Barrier internal electric field F_b (MV/cm)	0.64
Band discontinuity ΔE_c (meV)	376.5
Electron effective mass m^* (m_0) [39]	$0.23 + 0.05x$
Dielectric constant ϵ (ϵ_0) [39]	$8.1 + 1.5x$
Total polarization P_{tot} (C/m ²) [39]	$0.032x$
Intrasubband relaxation time τ_{in} (ps) [39]	0.24
Incident field's intensity I_L (W m ⁻²) [39]	1×10^{10}
Energy bandgap E_g (eV) [43]	$3.37 + 2.51x$
Superficial carrier density n_d (cm ⁻²) [44]	8.5×10^{11}

2.2. Non-Resonant Intense Laser Field (ILF) and Schrödinger Equation

In the presence of a non-resonant intense laser field (ILF), the interaction between the confined electron in the heterostructure and the incident electromagnetic field can be treated semi-classically, making use of the Kramers-Henneberger transformation, which transfers the time-dependence of the Hamiltonian to the confinement potential through an oscillating argument (gillcorralesstesis). Considering a high frequency incident field compared to the proper frequencies for the system's transitions, the time-dependent effect of the potential can be turned into a laser-dressed potential obtained by the period average of the oscillating potential. In this context, the Schrödinger equation for the electron in the QW, under the envelope function approximation, is given by [40],

$$-\frac{\hbar^2}{2} \frac{\partial}{\partial z} \left(\frac{1}{m^*(z)} \frac{\partial \psi_j(z, \alpha_0)}{\partial z} \right) + V(z, \alpha_0) \psi_j(z, \alpha_0) = E_j(\alpha_0) \psi_j(z, \alpha_0), \quad (4)$$

where $\hbar$ is the reduced Planck constant, $m^*(z)$ represents the effective mass varying along the z direction, and ψ_j, E_j are the wave function and energy associated with the j th state for the electron in the system. Under the mentioned approximation, the laser-dressed confinement potential V obtained from the interaction of the system with the external laser field is given by

$$V(z, \alpha_0) = \frac{1}{T} \int_0^T U[z + \alpha_0 \sin(\omega_0 t)] dt, \quad (5)$$

where α_0 is the dressing laser parameter and ω_0 is the non-resonant frequency of the laser field.

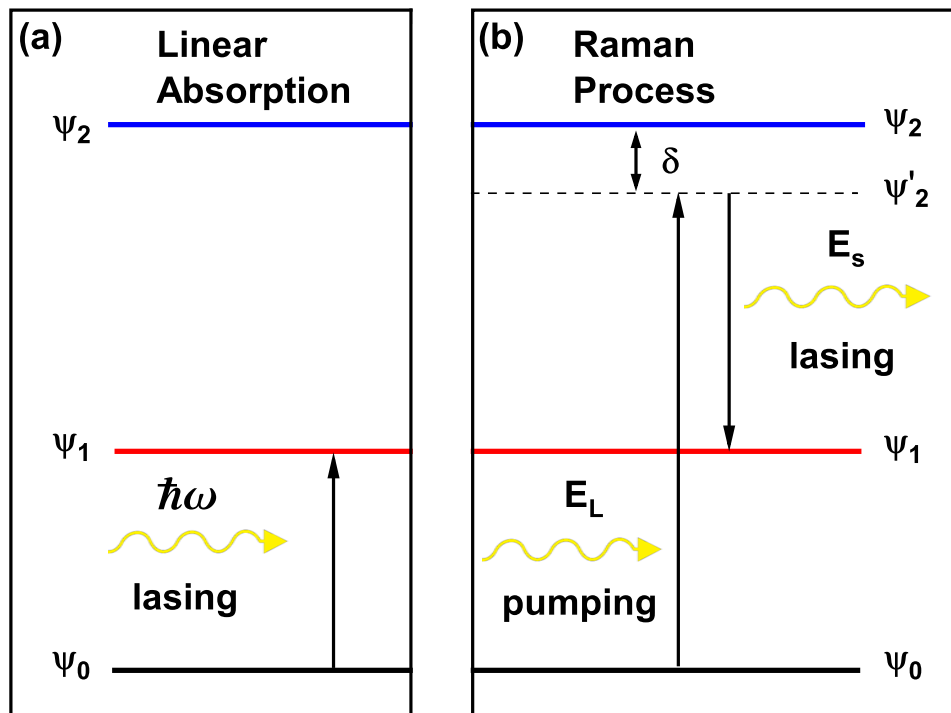


Figure 2. Transitions in the linear optical absorption and Raman process. In (a) is represented the states ψ_0 and ψ_1 for a given value of the incident photon's energy $\hbar\omega$. In (b) is depicted the Stokes Raman process of optical pumping from ψ_0 to a virtual state ψ'_2 due to the incident radiation E_L , and the lasing of secondary radiation E_s to reach ψ_1 , additional to the pump detuning δ between the real ψ_2 and virtual ψ'_2 states.

2.3. Linear Optical Absorption Coefficient and Temperature Dependence

The absorption of an incident photon's energy can produce a transition between ψ_i and ψ_j states (Figure 1(a)). This process in the system is modeled through a semi-classical interaction, where the quantum discrete states are the electronic states and the incident electromagnetic field exhibits classical

behavior, allowing each electron to interact with the field and be excited to higher energy levels. Employing a matrix density formalism combined with perturbation theory, it is possible to obtain an expression for the first order susceptibility (gilcorralestesis), and from this, the standard formula for linear optical absorption, which is given by [41]

$$\alpha_{ij}^{(1)}(\omega) = \hbar\omega \frac{\Lambda_{ij}}{\tau_{in}} \frac{|M_{ij}|^2}{(E_j - E_i - \hbar\omega)^2 + (\hbar/\tau_{in})^2}, \quad (6)$$

where $\Lambda_{ij} = \sqrt{\frac{\mu_0}{\epsilon_w \epsilon_0}} e^2 \sigma_{ij}$, ω is the frequency of the incident photon, $M_{ij} = \langle \psi_i | z | \psi_j \rangle$ is the transition matrix element and σ_{ij} the difference of volumetric carrier density between ψ_i and ψ_j states, respectively; τ_{in} is the intersubband relaxation time and ϵ_0, μ_0 are the vacuum permittivity and permeability, respectively.

Since the optical absorption depends on the volumetric carrier densities, it is important to understand and consider effects due to the laser-dressed potential and intensive properties, such as temperature, in the population of the ground and excited states. The total superficial carrier density n_d in the system is related to temperature through the superficial carrier density for the ψ_i state n_i as $n_d = \sum_{i=0}^2 n_i$, where n_i is given by [41]

$$n_i = \frac{m_w^*}{\pi \hbar^2} \int_{E_i}^{\infty} \frac{dE}{1 + \exp\left(\frac{E - E_f}{k_B T}\right)}, \quad (7)$$

where E_i is the energy of the ψ_i state, k_B is the Boltzmann constant, m_w^* is the well effective mass, and the relation between n_d and n_i is used to obtain the Fermi level E_f at temperature T . With the Fermi level known, the volumetric electronic population difference between states i and j σ_{ij} can be calculated as,

$$\sigma_{ij} = \frac{m^* k_B T}{\pi \hbar^2 L} \ln \left(\frac{1 + \exp[(E_f - E_i)/(k_B T)]}{1 + \exp[(E_f - E_j)/(k_B T)]} \right). \quad (8)$$

2.4. Raman Gain Theory

For scattering in general, an important concept is the differential cross section (DCS), which for the case of the Raman scattering is given by [40]

$$\frac{d^2\sigma}{d\Omega d\nu_S} = \Theta(\nu_L, \nu_S) W(\nu_S, \hat{u}_S), \quad (9)$$

where σ is the cross section, Ω is the solid angle, $\Theta(\nu_L, \nu_S) = \frac{V^2 \nu_S n(\nu_S)}{8\pi^3 c^4 n(\nu_L)}$, c is the vacuum speed of light, $n(\nu_{L,S})$ are the frequency-dependent refractive indexes, which can be considered equal; ν_L is the frequency of the incident radiation, ν_S is the frequency of the secondary radiation emitted, $\hat{u}_S$ is the polarization vector for the emitted secondary radiation field, $V = \frac{2}{\sigma_{01}}$ is the volume of the QW.

The Raman process considers two transitions: $\psi_0 \rightarrow \psi_2$ of absorption and $\psi_2 \rightarrow \psi_1$ of emission (Figure 1(b)), for which the transition rate $W(\nu_S, \hat{u}_S)$ is [40]

$$W(\nu_S, \hat{u}_S) = \frac{2}{\hbar} \frac{\mathcal{T}_{021}^2}{(E_s + E_1 - E_2)^2 + \Gamma_a^2} \times \frac{\Gamma_f}{(E_L - E_s + E_0 - E_1)^2 + \Gamma_f^2}, \quad (10)$$

where $\mathcal{T}_{021} = \langle \psi_0 | H_L | \psi_2 \rangle \times \langle \psi_1 | H_S | \psi_2 \rangle$ and Γ_a, Γ_f are the broadenings of the intermediate and final states, which are chosen to be $\Gamma_a = \Gamma_f = 5$ meV [33]. Since the problem is in one dimension,

the polarization vector for both the incident and the emitted secondary radiation can be taken as $\hat{u}_L = \hat{u}_S = (1, 0, 0)$ in the z -axis, and then, the photon-electron interaction operators H_k are given by

$$H_k = -\frac{i|e|\hbar}{m_0} \sqrt{\frac{2\pi\hbar^3}{Vv_k}} \frac{\partial}{\partial z}. \quad (11)$$

The magnitude of the differential cross section can be explained in terms of the expected value of the velocity operator $P_{ij} = \langle \psi_i | \frac{\partial}{\partial z} | \psi_j \rangle$ between the ψ_i and ψ_j state and the second order matrix element $T_{021}^2 = P_{02}^2 P_{12}^2$.

On the other hand, another important concept is the Raman gain, which is a quantity that characterizes the efficiency of the Raman scattering process for obtaining coherent emerging radiation. For the formula of gain to be obtained, it's needed to calculate the nonlinear susceptibility $\chi^{(3)}$ given by [40]

$$\chi^{(3)}(E_S, E_L) = -i \frac{\sigma_{01} |M_{02}|^2 |M_{12}|^2}{\epsilon_0 [(E_2 - E_0 - E_L)^2 + \Gamma^2] \Gamma}. \quad (12)$$

From this, the Raman gain can be obtained using

$$G_R(E_S, E_L) = -\frac{\omega_S}{n c} \text{Im} \left(\chi^{(3)}(E_S, E_L) \right) |\mathcal{E}|^2, \quad (13)$$

where $n = \sqrt{\epsilon_w}$ is the refractive index, ω_S is the frequency of the secondary radiation, $\Gamma = \hbar/\tau_{\text{in}}$ is the linewidth of the susceptibility [39], and $\mathcal{E}$ is the amplitude of the pumping or incident field which can be related with its intensity $I_L = 1 \times 10^{10} \text{ W m}^{-2}$ [39] by $|\mathcal{E}|^2 = \frac{2I_L}{nc\epsilon_0}$.

The energy of the incident field E_L can take a wide spectrum of values. It can be given by the physical process of electron excitation, in which it is supposed that the electron is pumped into a virtual state ψ'_2 with energy E'_2 from the ground state, before lasing the secondary radiation [42]. This E'_2 is related to the real state energy E_2 through the detuning $\delta = E_2 - E'_2 = E_2 - E_0 - E_L = 5 \text{ meV}$ by which a value of $E_L = \max\{E_2 - E_0\} - \delta$ is obtained.

3. Results

Figure 3 shows the conduction band bottom profile for a ZnO quantum well with length $L_w = 6 \text{ nm}$, with equal $\text{Mg}_{0.2}\text{Zn}_{0.8}\text{O}$ barriers of $L_b = 8 \text{ nm}$, additionally, the effects of the internal electric fields F_w and F_b are included in both the barrier and well regions. In this system, the effect of an intense non-resonant laser field determined by the dressing parameter α_0 has been included. Figure 3(a) compares the modification of the potential profile of the system initially without a laser field (black curve), with a laser parameter $\alpha_0 = 1 \text{ nm}$ (red curve) and for $\alpha_0 = 3 \text{ nm}$ (blue curve).

The potential modified by the effect of the intense laser field has been calculated according to Equation (5) and modifications are evident in the interfaces between both materials with a curved characteristic, which is a typical effect of the response to an intense non-resonant laser field, also, note the decrease in the depth of the central well that is proportional to the magnitude of the dressing parameter (compare the well region for $\alpha_0 = 1 \text{ nm}$ and $\alpha_0 = 3 \text{ nm}$). The mentioned modifications originate particular changes in the limited states of the system that imply a potential control in the optical properties, as will be mentioned later. This laser-induced symmetry directly affects the dipole matrix elements and, consequently, the allowed optical transitions.

Figure 3(b) shows the energy variation as a function of the laser parameter α_0 for the first three confined states in the quantum well system with $L_w = 6 \text{ nm}$ for the well and $L_b = 8 \text{ nm}$ for the barriers. The ground state is represented by the black line, and the first and second excited states are represented by the red and blue lines, respectively, and the Fermi level is shown in dashed lines.

As the laser parameter increases, the bottom of the quantum well shifts toward higher energies, as shown in Figure 3(a), this results in a blue shift of the energy levels, and the most affected state is the ground state since it is located closer to the bottom of the well. In the range of variation of the laser parameter $0.0 < \alpha_0 < 3.0$, the ground state varies approximately within $174 \text{ meV} < E_0 < 286 \text{ meV}$.

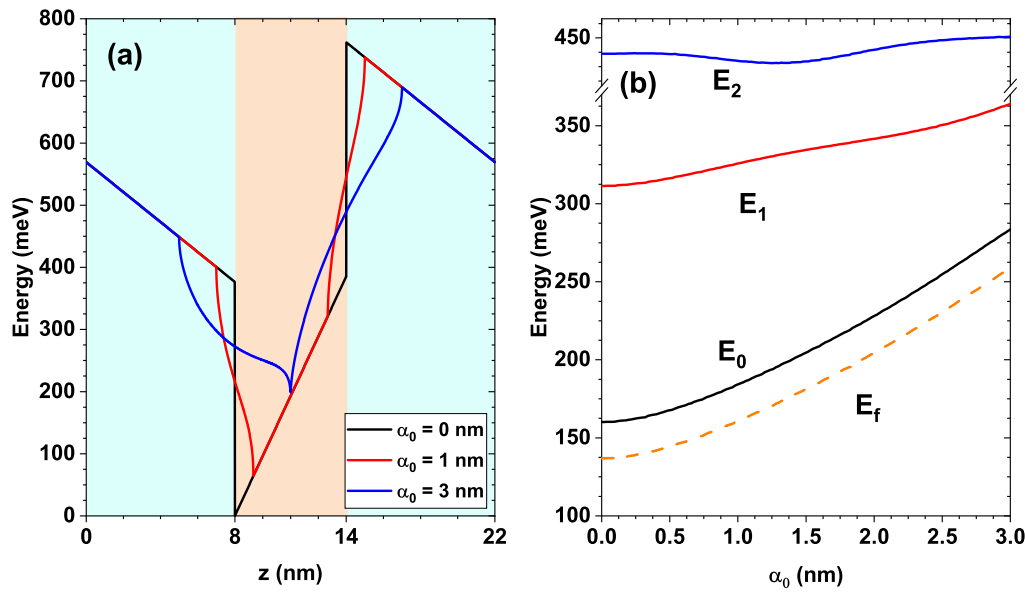


Figure 3. In (a), variation of the dressed confinement potential V along position on z -axis in a $\text{ZnO}/\text{Mg}_{0.2}\text{Zn}_{0.8}\text{O}$ QW system with dimensions $L_w = 6$ nm for the well and $L_b = 8$ nm for the barriers. Different values of the dressing parameter $\alpha_0 = 0$ nm, 1 nm and 3 nm are considered. In (b), variation of the energies for ground stated E_0 , first E_1 and second E_2 excited states, and Fermi level E_f (dashed line) depending on the dressing parameter α_0 in a $\text{ZnO}/\text{Mg}_{0.2}\text{Zn}_{0.8}\text{O}$ QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm.

Note that as α_0 increases, the energy separation between the ground state and the first excited state decreases (see the black and red curves in Figure 3(b)). The same behavior occurs for the separation between the first and second excited states (see the red and blue curves in Figure 3(b)). This is because the ground state tends to increase its energy along with the bottom of the well. However, this effect is compensated for by the fact that the well also increases its average width, causing the higher-energy states to shift downward, thus becoming closer in energy.

Figure 4 shows the wave functions of the first three confined states in the quantum well: the ground state ψ_0 (black curve), and the first and second excited states ψ_1 and ψ_2 (red and blue curves, respectively), for four different values of the laser parameter: $\alpha_0 = 0$ in panel (a), $\alpha_0 = 1$ nm in panel (b), $\alpha_0 = 1.36$ nm in panel (c), and $\alpha_0 = 3$ nm in panel (d). The dashed line in each panel corresponds to the maximum value of the wave function associated with the ground state, this line has been included to analyze the symmetry of the states as the laser parameter increases.

In Figure 4(a), the system does not include the laser field effect ($\alpha_0 = 0$), and the shapes of the wave functions are determined solely by the confinement potential of the structure. Note that the ground state exhibits a shift toward the left, caused by the asymmetry of the triangular-shaped well, as shown in Figure 3(a) (black curve). Evidently, this lack of parity is also reflected in the first and second excited states. Clearly, the ground state is not an even function, as indicated by the absence of symmetry with respect to the vertical dashed line located at its maximum value. This feature has consequences for the associated optical properties, as will be discussed later.

Figure 4(b) shows the same states for a laser field of $\alpha_0 = 1$ nm, whose associated potential is depicted in Figure 3(a) (red curve), note that the ground state and the first excited state tend to behave as even states (see the black and red curves). This behavior is not observed for the second excited state (blue curve). In Figure 4(c), the laser parameter for which the wave functions reach their point of maximum symmetry is shown (for $\alpha_0 = 1.36$ nm). This result can be corroborated through the calculation of the dipole matrix elements between the states, as illustrated in a later figure.

This behavior can be explained by the fact that the laser field induces a modification in the bottom of the potential, transforming it from a sawtooth-like profile (clearly asymmetric) into a V-shaped potential (symmetric), thereby inducing a local parity in the lowest states of the system. In Figure 4(d),

for a laser parameter of $\alpha_0 = 3$ nm, the previously mentioned local symmetry is broken again (as seen in Figure 3(a), blue curve), causing the lowest states to lose their parity once more.

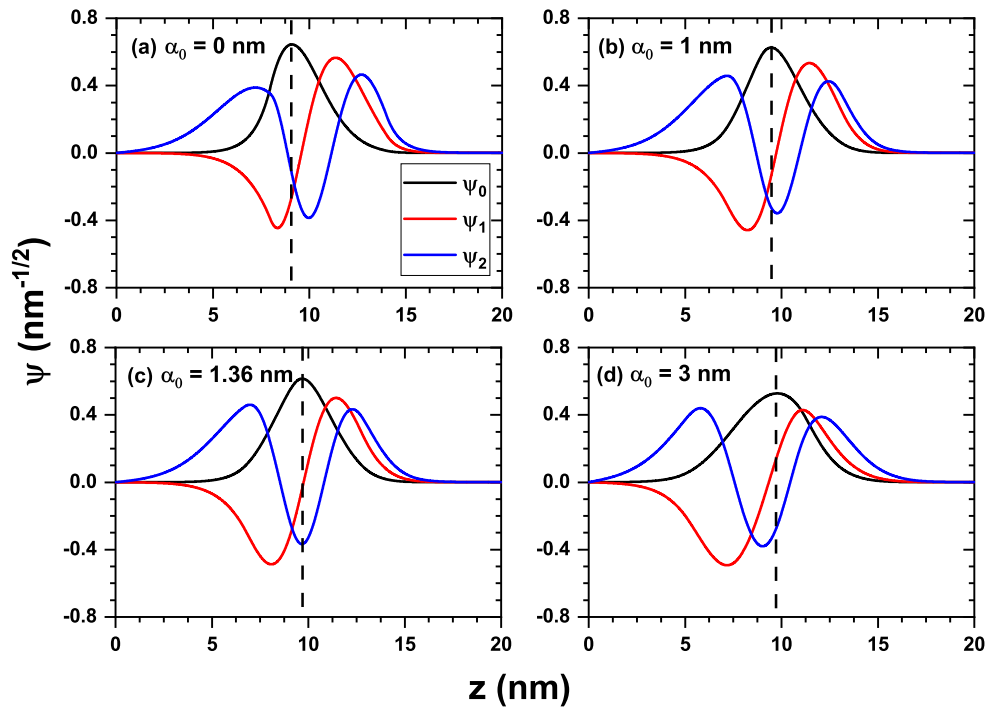


Figure 4. Normalized wave functions for the first three states for a ZnO/Mg_{0.2}Zn_{0.8}O QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm, depending upon different values of the dressing parameter α_0 . The dashed line represents the point of maximum amplitude for the wave function ψ_0 in each of the values for α_0 . In (a), the dressing parameter value taken is $\alpha_0 = 0$ nm, while in (b) the parameter is taken as $\alpha_0 = 1$ nm. The value in (c) is obtained by the cancellation of the matrix element M_{02} , which gives $\alpha_0 = 1.36$ nm. In (d), the last value considered for the parameter is $\alpha_0 = 3$ nm.

Figure 5 shows the integrand of the dipole matrix element $\psi_0 z \psi_2$ as a function of the position z for four different values of the non-resonant intense laser parameter: $\alpha_0 = 0$, $\alpha_0 = 1$ nm, $\alpha_0 = 1.36$ nm, and $\alpha_0 = 3$ nm, corresponding to Figures 5(a), 5(b), 5(c), and 5(d), respectively. Each figure presents the corresponding value of the squared dipole integral $|M_{02}|^2$, the highest value occurring for $\alpha_0 = 0$, where a clear asymmetry is observed in the local maxima of the curve (see Figure 5(a)). Subsequently, a significant decrease in the value is observed for $\alpha_0 = 1$ nm, where the local maxima reach similar values (Figure 5(b)). Figure 5(c) shows that the matrix element is equal to zero for $\alpha_0 = 1.36$ nm, canceling the integral value despite the fact that the two local maxima of the curve clearly reach different values. This is a characteristic of the potential asymmetry, where the area under the curve corresponding to the two maxima has the same magnitude as the area of the relative minimum. The cancellation of the integral arises from the compensation between the positive and negative contributions of the wave functions due to their spatial symmetry. Finally, for $\alpha_0 = 3$ nm, the matrix element again takes nonzero values, and the asymmetry of the system becomes more evident.

Figure 6(a) shows the linear optical absorption coefficient associated with the transition between the ground state and the first excited state, α_{01} , for three different values of the laser parameter: $\alpha_0 = 0$, $\alpha_0 = 1$ nm, and $\alpha_0 = 3$ nm (black, red, and blue curves, respectively). Note that the peak corresponding to $\alpha_0 = 0$ is around 150 meV, which is consistent with the transition energy $\hbar\omega = E_1 - E_0 \approx 150$ meV (see Figure 3, black and red curves). The magnitude of the absorption coefficient is proportional to the matrix element $|M_{01}|^2$, as shown in Equation (6), and its behavior as a function of the laser parameter is presented in Figure 6(b).

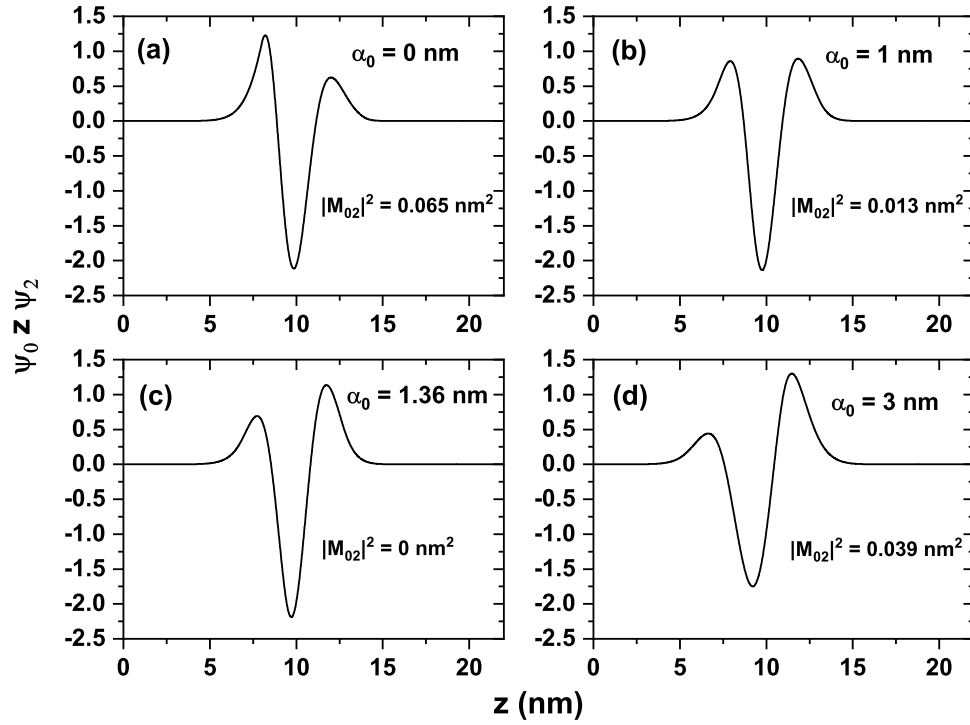


Figure 5. Argument of the matrix element integral $\psi_0 z \psi_2$ plotted versus position z in the system for a ZnO/Mg_{0.2}Zn_{0.8}O QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm, considering different values for the dressing parameter α_0 . In (a) is depicted the argument for $\alpha_0 = 0$ nm, in which the left peak is higher than the right peak. In (b), the peak's heights are equal for both left and right. In (c) and (d), this characteristic is inverted, since the right peak increases in height while the left peak decreases.

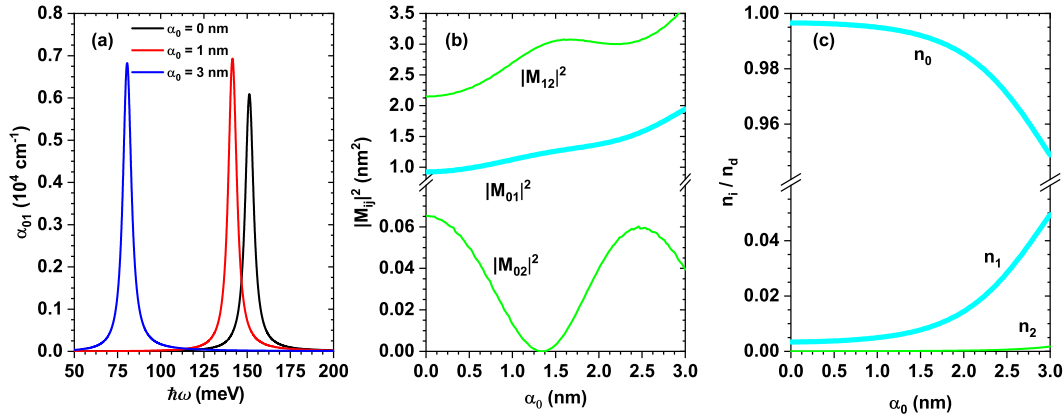


Figure 6. In (a), absorption coefficient α_{01} in the given ZnO/Mg_{0.2}Zn_{0.8}O QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm, depending upon the incident photon's energy $\hbar\omega$ of the resonant laser for different values of α_0 . In (b), matrix elements $|M_{ij}|^2$ depending on the variation of the dressing parameter α_0 for ψ_0 , ψ_1 and ψ_2 states in the given ZnO/Mg_{0.2}Zn_{0.8}O QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm. In (c), normalized carrier density per unit area n_i/n_d for the ψ_0 , ψ_1 and ψ_2 states in the given ZnO/Mg_{0.2}Zn_{0.8}O QW system with dimensions $L_w = 6$ nm and $L_b = 8$ nm.

The red curve corresponds to $\alpha_0 = 1$ nm and exhibits a maximum at approximately 143 meV, which agrees with the energy difference between the states E_0 and E_1 for this value of the laser parameter (see Figure 3(b)). Note that this peak has a larger magnitude than the one corresponding to $\alpha_0 = 0$. This is due to the fact that the associated matrix element $|M_{01}|^2$ increases with the laser parameter, as shown in Figure 6(b) in the highlighted $|M_{01}|^2$ curve.

Finally, the linear absorption curve for $\alpha_0 = 3$ nm (blue curve) reaches its maximum around 80 meV, which corresponds to the point where the states E_0 and E_1 are closest, as observed in the energy curve. The magnitude of this curve is slightly smaller than that for $\alpha_0 = 1$ nm, despite the fact that the

matrix element reaches a higher value (on the order of 2 nm^2), according to Figure 6(b). This reduction is caused by the electronic population difference between the corresponding states, $\sigma_{01} = n_0 - n_1$, which is also proportional to the linear absorption coefficient. Figure 6(c) shows this behavior, where it is evident that for $\alpha_0 = 0$ and $\alpha_0 = 1 \text{ nm}$ the population difference remains very similar (with a clearly high occupation of the ground state); thus, in these cases the magnitude of the absorption is mainly determined by the matrix element $|M_{01}|^2$. However, for $\alpha_0 = 3 \text{ nm}$ the population difference reaches a minimum value, which explains the decrease in the corresponding absorption coefficient (for this value of the laser parameter, the electronic occupation of the ground state decreases slightly, and a relevant occupation of the first excited state begins to emerge).

Figure 7 shows the DCS (see equation (9)) for the same previously fixed geometry and two different values of the laser pumping field, $E_L = 276.61 \text{ meV}$ (Figure 7(a)) and $E_L = 400 \text{ meV}$ (Figure 7(b)). The first value corresponds to the resonance energy between the second excited state and the ground state ($E_2 - E_0 - \delta \approx 276.61 \text{ meV}$ for $\alpha_0 = 0$). The second value of E_L is much larger than this resonance in order to ensure proper excitation of the states involved. To better understand the behavior in Figures (a) and (b), Figure 7(c) has been included, showing the second-order matrix element T_{021} , which is proportional to the DCS.

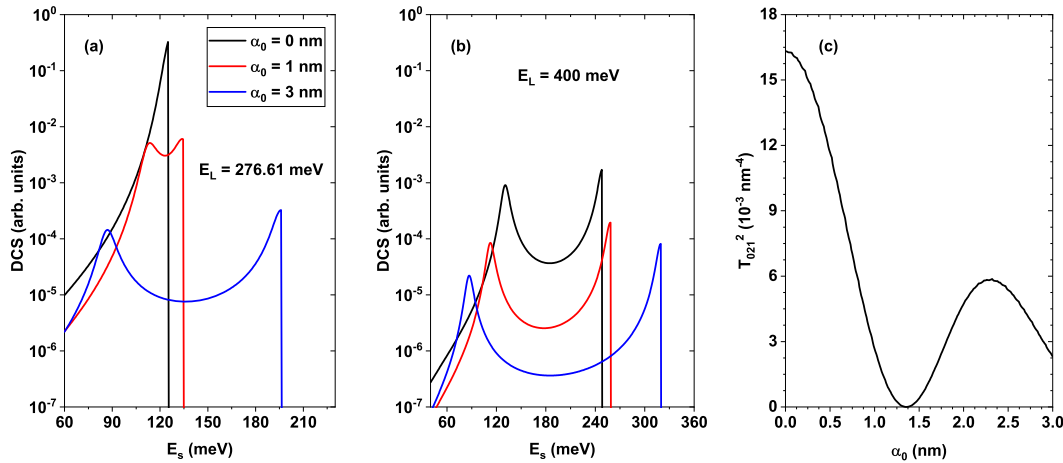


Figure 7. Raman differential cross section (DCS) in a $\text{ZnO}/\text{Mg}_{0.2}\text{Zn}_{0.8}\text{O}$ QW with dimensions $L_w = 6 \text{ nm}$ and $L_b = 8 \text{ nm}$ depending on the emitted radiation energy E_s and different values of the dressing parameter α_0 . In (a), the value for the incident laser energy is taken as $E_L = 276.61 \text{ meV}$, given by the detuning $\delta = 5 \text{ meV}$ for the Raman transition process to the virtual state. In (b), the energy value for the incident laser is taken as $E_L = 400 \text{ meV}$ for comparison. The picture in (c) shows the second order matrix element T_{021} depicted as a function of the dressing parameter α_0 .

The DCS must generate two peaks (resonant like and step like) because it is proportional to the transition rate, which is the product of two Lorentzian functions whose maxima are located at the positions $E_s = E_2 - E_1$ and $E_s = E_L - (E_1 - E_0)$ according to equation (10). When $E_L = 276.61 \text{ meV}$ (resonance point) and $\alpha_0 = 0$, the two maxima of the Lorentzian profiles are very close, differing only by a factor $\delta = 5 \text{ meV}$. With the value of Γ used, the DCS behaves as a single peak with a value of approximately 125 meV (see the blue and red curves in Figure 3(b)), as shown in Figure 7(a), black curve. This curve also exhibits a greater magnitude compared to the others, as the matrix element T_{021} reaches a maximum value for $\alpha_0 = 0$, as can be seen in Figure 7(c).

For $\alpha_0 = 1 \text{ nm}$ (red curve in Figure 7(a)), two DCS peaks can already be resolved because the first resonance is located at the new position $E_s = E_2 - E_1 \approx 102 \text{ meV}$ and the second at $E_s = E_L - (E_1 - E_0) \approx 276.61 - \delta - 147.5 = 124.1 \text{ meV}$, with a smaller magnitude, as evidenced in the curve T_{021} in Figure 6(c) for $\alpha_0 = 1 \text{ nm}$. These transition energy values can be verified in Figure 3(b). A similar situation occurs for $\alpha_0 = 3 \text{ nm}$, where the DCS peaks are much farther apart because the resonances are now at $E_s = E_2 - E_1 \approx 87.5 \text{ meV}$ and $E_s = E_L - (E_1 - E_0) \approx 276.61 - \delta - 81.3 = 190.3 \text{ meV}$,

respectively, and with an even lower magnitude for this value of the laser parameter, as can be seen from the T_{021} curve.

In Figure 7(b), the DCS and the peaks are much more clearly defined because the energy E_L is far from the resonance energy between the states involved (significant detuning), allowing better resolution of the Raman peaks. However, the magnitude of these peaks decreases strongly because of the increase in the denominator of the Lorentzian functions in the transition rate. These results demonstrate the possibility of tuning the position and magnitude of the Raman peaks in ZnO/MgZnO quantum wells through modifications in the characteristics of the non-resonant external laser field, which is essential for practical applications.

Figure 8 shows the Raman gain calculated from equation (13) as a function of the laser parameter for the two values of E_L : 276.61 meV, which corresponds to the resonant case in Figure 8(a), and 400 meV, which corresponds to the off-resonant case in Figure 8(b). In the first case, Figure 8(a), we have $E_L = (E_2 - E_0)_{\alpha_0=0} - \delta$, with this expression in the denominator of susceptibility, it takes the form $((E_2 - E_0) - (E_2 - E_0)_{\alpha_0=0} + \delta)^2 + \Gamma^2$, for $\alpha_0 = 0$, it becomes $\delta^2 + \Gamma^2$. As the laser parameter increases, the term $E_2 - E_0$ becomes smaller, reducing the denominator of susceptibility and increasing the gain, until it reaches a maximum value obtained when $E_2 - E_0 = (E_2 - E_0)_{\alpha_0=0} - \delta$ for approximately $\alpha_0 = 0.34$ nm. From this point on, the susceptibility denominator starts to increase, reducing the gain, as seen in Figure 8(a). The gain is also proportional to the product of the matrix elements $|M_{02}|^2 |M_{12}|^2$, whose behavior is shown in Figure 6(b). This product becomes zero at approximately $\alpha_0 = 1.4$ nm and reaches a new maximum for α_0 between 2 nm and 2.5 nm, as evidenced in the inset of Figure 8(a).

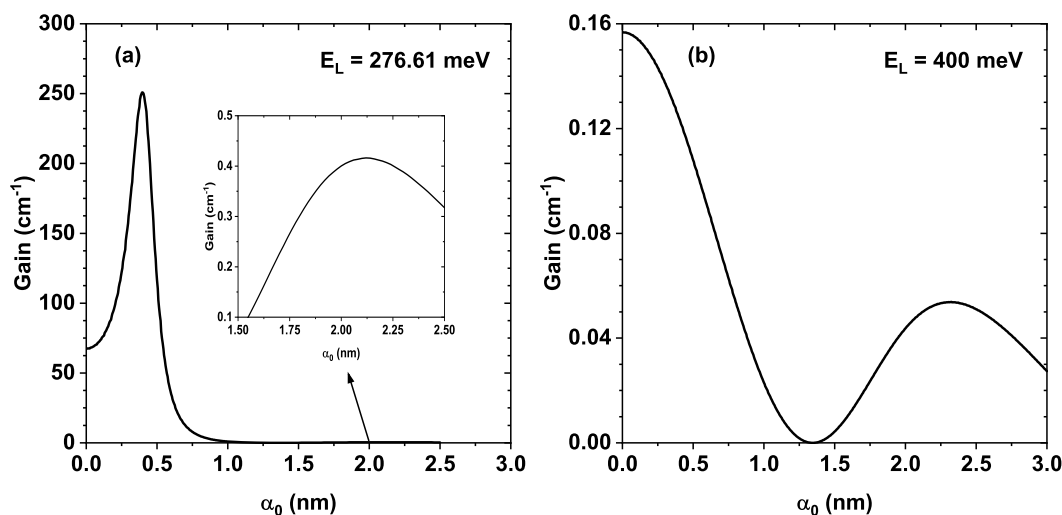


Figure 8. Raman gain for a electron in the the given ZnO/Mg_{0.2}Zn_{0.8}O QW system whose dimensions are $L_w = 6$ nm and $L_b = 8$ nm as function of the parameter α_0 . In (a), the energy for the pumping laser is $E_L = 276.61$ meV, which is obtained considering the detuning δ for the Raman transition; here, the gain curve is shown in a thinner range for α_0 in which it is seen to have a dominant and well defined peak near $\alpha_0 = 0.4$ nm. In (b), the energy for the pumping laser is taken as $E_L = 400$ meV and the curve, shown for the whole range for α_0 is seen to have much less magnitude as in (a) and a very different form.

Figure 8(b) shows the Raman gain but now for $E_L = 400$ meV, that is, an energy much higher than the resonance energy of the system. This increase causes the term $(E_2 - E_0 - E_L)^2$ in the denominator of the gain to take very large values, producing a decrease throughout the entire range of the laser parameter. This explains the significant difference in magnitude between Figure 8(a) and Figure 8(b). In this figure (b), two local maxima are observed for $\alpha_0 = 0$ and approximately at $\alpha_0 = 2.4$ nm, which coincide with the local maxima of the matrix element $|M_{02}|^2$ in Figure 6(b). Note that the position of the gain minimum located near approximately 1.4 nm is also predicted.

In the resonant case (Figure 8(a)), the laser parameter can significantly modify the Raman gain in this system, increasing it from approximately 65 cm^{-1} to nearly 250 cm^{-1} as the parameter varies from

0 to 0.4 nm, that is, almost four times the initial magnitude. However, the magnitude of the Raman gain can also be controlled through the external pumping laser. This implies that the Raman gain in this system is not a fixed quantity; it can be tuned by external fields, which is useful for potential applications in field-dependent optoelectronic devices, quantum gain modulators, or controlled Raman amplifiers.

4. Conclusions

In this work, we investigated the effects of a non-resonant intense laser field on the optical absorption and Raman scattering processes in ZnO/Mg_{0.2}Zn_{0.8}O quantum wells by analyzing the modifications induced in the confinement potential, electronic structure, transition matrix elements, and nonlinear optical response, these types of heterostructure give rise to internal electric fields that have also been modeled. Our results demonstrate that the dressing parameter α_0 , which characterizes the strength of the external laser field, introduces significant and highly tunable modifications to both the energy levels and the spatial distribution of the confined electronic states. These laser-induced alterations lead to pronounced shifts in intersubband transition energies, symmetry-driven changes in the dipole matrix elements, and a strong redistribution of carrier populations.

The interplay between these effects results in substantial tailoring of the linear optical absorption coefficient and the Raman response. In particular, the Raman differential cross section exhibits controllable peak positions and magnitudes, directly related to the behavior of the second-order matrix element T_{021} . Likewise, the Raman gain shows a remarkable sensitivity to the laser field: under resonant pumping conditions, the gain can be enhanced by nearly a factor of four for moderate values of α_0 , whereas in the non-resonant scenario the overall magnitude is strongly suppressed but still retains a field-dependent structure associated with the matrix-element modulation.

These findings demonstrate that the optical response of ZnO/MgZnO quantum wells is not a fixed property of the heterostructure but can be efficiently tuned by external non-resonant laser fields. The ability to modulate absorption, Raman scattering, and Raman gain through an accessible control parameter suggests promising opportunities for the design of field-dependent optoelectronic devices, tunable Raman amplifiers, quantum gain modulators, and other photonic technologies based on wide-bandgap oxide semiconductors.

Author Contributions: The contributions of the authors are as follows: S.U.-P.: Conceptualization, Methodology, Software, Validation, Formal Analysis, Investigation, Data curation, Writing—Review and Editing. J.A.G.-C.: Conceptualization, Methodology, Software, Validation, Formal Analysis, Investigation, Data curation, Writing—Review and Editing. J.A.V.: Conceptualization, Writing—Review and Editing, Visualization. A.L.M.: Conceptualization, Formal Analysis, Writing—Review and Editing, Visualization. C.A.D.: Conceptualization, Formal Analysis, Writing—Review and Editing, Visualization. All authors have read and agreed to the published version of the manuscript.

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