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Analysis of the influence of external magnetic field on transition matrix elements in quantum well and quantum cascade laser structures

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ABSTRACT

We present a method for modeling nonparabolicity effects (NPE) in quantum nanostructures in presence of external electric and magnetic field by using second order perturbation theory. The method is applied to analysis of quantum well structure and active region of a quantum cascade laser (QCL). This model will allow us to examine the influence of magnetic field on dipole matrix element in QCL structures, which will provide a better insight to how NPE can affect the gain of QCL structures.

1. Introduction

Nonparabolicity effects (NPE) in the conduction band (CB) of a semiconductor quantum well (QW) material have an essential role in modeling of electronic structure of multiple QW structure such as quantum cascade laser (QCL). By using 14-band **kp** calculation presented in [1], Ekenberg in [2] determined the coefficients in the expansion of the dispersion relation up to the fourth order in wavevector. This results in a forth order differential equation with boundary conditions obtained by double integration, which fulfill the requirement for probability current conservation [3]. In [4] the authors presented the model from [2,3] and its application to QCL structures by using transfer matrix method (TMM). Modeling of NPE mathematically represents a nonlinear eigenvalue problem, thus it is preferable to develop an approximate solution.

QCL structures are powerful light sources emitting from mid-infrared (MIR) to THz frequencies that have turned out to be efficient and reliable in free-space communications, medical diagnostics, and chemical sensing [5–9]. By engineering of the active region, it is possible to obtain wide scope of operating wavelengths from 3 μm up to 360 μm [10,11]. The lasing wavelength is defined by separation of laser energy states, and for THz frequencies the energy difference is very small (around 10 meV) and thus any shift in energy can make modeling of these structures more demanding.

Development of THz QCL structures also included application of external magnetic field due to the interest to cover lower frequencies and allow better temperature performance [12–14]. Application of magnetic field causes Landau discretization of energy states in QCL which suppresses non-radiative intersubband scattering and allows significant decreasing in threshold current [15], operation on low frequencies [16] and on higher temperatures [17]. Due to the increased gain and lower threshold, application of magnetic field can highly improve QCLs which don't perform well without it. This allows possibility

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for experimental confirmation without growth challenging proposals based on quantum dot superlattices. This allows possibility for experimental confirmation without growth challenging proposals, with expected formation of strongly coupled electron-phonon polarons, based on quantum dot superlattices [18–20].

Performance of magnetic field assisted structures can be even more enhanced in non-GaAs/AlGaAs structures such as InGaAs/GaAsSb [21] and InGaAs/AlInGaAs [22] where NPE are stronger due to the lower band gap which raises the significance of their modeling.

In this paper we use the model from [2–4] and apply the second order perturbation theory in order to model energy corrections more accurately. In [2], Ekenberg applied first order perturbation theory for energies and authors in [4] only used unperturbed Hamiltonian from [2], while in this paper we will present a more precise treatment through the second order perturbation theory. We will apply this model to QW structure without the presence of external electric field which yields analytic solution, and then consider QCL structure for which this model can have a great importance. We will also consider the first order correction for the wavefunctions and this will allow us to study the effect of magnetic field on dipole matrix element, or in another sense, on the gain of QCL.

2. Theoretical consideration

We will focus on the Hamiltonian given in [2] in the presence of magnetic field, which can be written as

$$
\begin{aligned}
\widehat{H} &= \widehat{H}_{NP0} + \widehat{H}_{NP} \\
\widehat{H}_{NP0} &= \widehat{H}_0 + \widehat{H}' \\
\widehat{H}_{NP} &= (2\alpha_0(z) + \beta_0(z))^* \frac{1}{2}\left\{\widehat{k}_x, \widehat{k}_y\right\}^2 + \alpha_0(z)\left(\widehat{k}_x^4 + \widehat{k}_y^4\right) \\
\widehat{H}_0 &= \widehat{k}_z^2 \alpha_0(z) \widehat{k}_z^2 + \frac{\hbar^2}{2}\widehat{k}_z \frac{1}{m^*(z)} \widehat{k}_z + V(z) \\
\widehat{H}' &= \left(j + \frac{1}{2}\right)\widehat{\left(\frac{1}{M(z)}\right)} eB\hbar \\
\widehat{\left(\frac{1}{M(z)}\right)} &= \frac{1}{m^*(z)} + \frac{2}{\hbar^2}\widehat{k}_z(2\alpha_0(z) + \beta_0(z))\widehat{k}_z
\end{aligned}
\tag{1}
$$

Here, $\widehat{H}_{NP0}$ represents the part of the Hamiltonian $\widehat{H}$, *i.e.* $\widehat{H}_{NP0} = \widehat{H}\left(\widehat{k}_{||} = 0\right)$. $\widehat{H}_{NP}$ can be treated with the second order perturbation theory (first correction vanishes) and this was done in [2]. In this paper we focus on $\widehat{H}_{NP0}$, and apply the second order perturbation theory. Hence $\widehat{H}_{NP0}$ can be represented as a sum of unperturbed Hamiltonian $\widehat{H}_0$ and the perturbed one $\widehat{H}$'. The coefficients α_0 and β_0 are nonparabolicity parameters given in [2], B is the magnetic induction of external magnetic field, $V(z)$ is the potential of the structure, $\widehat{k}_x, \widehat{k}_y, \widehat{k}_z$ are the wavevector components operators, $m^*(z)$ is the effective mass at the bottom of conduction band and j is the Landau level index.

The Hamiltonian in (1) operates on envelope wavefunction $\eta_n(z)$ and we treat $\widehat{H}_{NP0}$ and $\widehat{H}_{NP}$ separately. For $\widehat{H}_{NP0}$ we first solve the eigenvalue problem with unperturbed Hamiltonian $\widehat{H}_0\eta_{n0} = E_n^{(0)}\eta_{n0}$ (index 0 denotes unperturbed values, while $n = 1,2, \ldots$ represent bound state energy indices) and use the wavefunctions $\eta_{n0}(z)$ as a basis for perturbation theory. First order correction for energy is given in [2] as

$$
\begin{aligned}
\Delta E_n^{(1)} &= \left(j + \frac{1}{2}\right)\frac{eB\hbar}{m_{||}} \\
\frac{1}{m_{||}} &= \int_{-\infty}^{\infty} \eta_{n0}^* \widehat{\left(\frac{1}{M(z)}\right)} \eta_{n0} dz
\end{aligned}
\tag{2}
$$

Second order correction for energy can be determined as

$$
\begin{aligned}
\Delta E_n^{(2)} &= \left[\left(j + \frac{1}{2}\right)eB\hbar\right]^2 \sum_{k \neq n} \frac{|M_{nk}|^2}{E_n^{(0)} - E_k^{(0)}} \\
M_{nk} &= \int_{-\infty}^{\infty} \eta_{n0}^* \widehat{\left(\frac{1}{M(z)}\right)} \eta_{k0} dz, \quad n \neq k
\end{aligned}
\tag{3}
$$