Correction to the Effective Refractive Index and the Confinement Factor in Waveguide Modeling for Quantum Cascade Lasers

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(Dated: 21 July 2021)

The equations for the effective medium refractive index and for the confinement factor in the waveguide design for quantum cascade lasers are derived. Compared to equations used in prior literature, by applying rigorous perturbation theory and including the effect of the anisotropic optical gain and non-Hermitian properties of the waveguide structure and materials, a few percent correction should be made to the confinement factor and the effective gain. This result can easily be generalized to any optical devices with a layered structure.

I. INTRODUCTION

Active semiconductor optical devices including LEDs, lasers, meta-material devices, etc. have been developing rapidly, introducing complex multi-layered optical structures. Concepts including the effective refractive index and the confinement factor\textsuperscript{1–3} are often used to simplify the modeling of those structures. One good example is quantum cascade lasers (QCLs)\textsuperscript{4}, where tens-of-atomic scale layers as quantum wells and multi-layered sub-wavelength optical claddings are built on a single wafer to produce efficient lasers of mid-infrared to THz light.

Since the invention of QCLs, much effort has been made to improve the laser performance, both via active region design and the waveguide design. Different waveguiding mechanisms including index guiding, plasmonic guiding, and double-metal waveguiding\textsuperscript{5,6} are widely used to reduce the optical loss of the device as well as to increase the confinement factor.

The confinement factor in particular has been defined differently in different references\textsuperscript{1–3,7–9}. To the best of our knowledge, there is not any published analytical analysis about what should be the more accurate equation for the effective medium refractive index and the confinement factor that takes into consideration the polarization selection law for QC gain, the particulars of QCL layer structures and the non-Hermitian property of lossy materials in the waveguide.

In this work, we derive the equations for the effective refractive index and the confinement factor directly from Maxwell’s equations, and discuss when conventional expressions often used in literature may lead to noticeable errors.

In Section II we define the model and the variables for the work; running wave effective refractive index in an infinite periodical structure is investigated in Section III to derive the effective medium refractive index in active core of a QCL, which is compared with numerical result to show the validity of the effective medium approxima-

\begin{align*}
\nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} &= \frac{\omega^2}{c^2} \mathbf{H} \\
\mathbf{E} &= \frac{i}{\omega \varepsilon_0} \nabla \times \mathbf{H}
\end{align*}

where $\varepsilon$ generally should be a symmetric tensor with complex elements, but we assume it to have a principle axis along the $x$, $y$ and $z$ direction, noted as $\varepsilon =$

\textbf{II. 1D MAXWELL’S EQUATIONS FOR A 2D WAVEGUIDE}

FIG. 1. The coordinate system: for sketch purposes we draw a ridge waveguide to show the direction of wave propagation. The 2D waveguide is a good approximation when the ridge width along $x$ is much larger than the wavelength. The refractive index profile varies in different waveguide designs, but usually includes cladding layers and periodical active layers (red).

In the following context we assume relative permeability $\mu = 1$; the relative permittivity $\varepsilon = n^2$ is a function of $y$, which is the growth direction of the epi-layers; the structure is constant and infinite in $x$ and $z$ direction, where the $z$ direction is the direction of wave propagation; see Fig. 1 for a diagram of the coordinates.

Maxwell’s equations at a frequency $\omega$ can be written as:

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Diag\{\varepsilon_x,\varepsilon_y,\varepsilon_z\} = Diag\{n_x^2, n_y^2, n_z^2\}. This is justified by the y-axial symmetry of the structure, and the fact that growth and fabrication most commonly happens along major crystal directions.

\[ \nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} = \begin{pmatrix}
-\partial_y \varepsilon_x^{-1} \partial_y + \beta^2 k^2 \varepsilon_y^{-1} & 0 & 0 \\
0 & 0 & 0 \\
-\beta k \varepsilon_y^{-1} & 0 & -i \beta k \partial_y \varepsilon_y^{-1} \partial_y
\end{pmatrix} \begin{pmatrix}
H_x \\
H_y \\
H_z
\end{pmatrix} \]

which is naturally block diagonal, giving modes \( H_y = H_z = 0 \) (transverse magnetic, TM) and \( H_x = 0 \) (transverse electric, TE). For the TM modes, which is the mode of QCLs due to the selection law for intersubband transition\[n\] the 3D equation reduces to 1D:

\[ \begin{align*}
( - \frac{\partial}{\partial y} \frac{1}{n_y^2} \frac{\partial}{\partial y} + \frac{\beta^2 k^2}{n_y^2} ) H_x &= \frac{\omega^2}{c^2} H_x \\
E_y &= -\frac{\beta k H_x}{\omega \varepsilon_0 n_y^2} \\
E_z &= -\frac{i}{\omega \varepsilon_0 n_z^2} \frac{\partial H_x}{\partial y}
\end{align*} \]

III. THE UNGUIDED EFFECTIVE REFRACTIVE INDEX IN THE ACTIVE REGION

The active region of QCLs typically consists of tens of periods of active and injection layers, consisting of multiple quantum wells and barriers, each of which are typically a few atoms thick, adding up to a period length of a few hundred angstroms. This period is about one order of magnitude smaller than the wavelength in vacuum, and therefore the effective medium theory is commonly applied. In this section we show, however, a more accurate expression for the effective refractive index for QCL active regions.

For an active region with period \( L_p \), assuming a structure with infinite number of periods, the Bloch theory gives \( H_x = u(y)e^{ikL_p} \), with \(-\pi/L_p < k \leq \pi/L_p\) and \( u(y+L_p) = u(y) \). In the frequency domain Eq. (4) is (for simplicity here we use the fact that within each individual quantum well and quantum barrier layer the material is isotropic, i.e. \( n_x = n_y = n_z = n \):

\[ u(y) = \sum_{j=-\infty}^{\infty} u_j e^{2\pi j y/L_p}, \]

\[ \frac{1}{n(y)^2} = \sum_{j=-\infty}^{\infty} \frac{1}{n_j^2} u_j^{2\pi j y/L_p}, \]

\[ \sum_q \left[ \frac{2\pi q}{L_p} + k \right] \left[ \frac{2\pi q}{L_p} + k + \beta^2 k^2 \right] \frac{u_q}{n_{j-q}^2} = \frac{\omega^2}{c^2} u_j \]

where \( u(y) \) is the slowly varying amplitude of the field, \( n(y) \) is the spatial dependent refractive index, \( u_j \) and \( 1/n_j^2 \) are Fourier series of \( u(y) \) and \( 1/n(y)^2 \), \( \beta \) is the effective refractive index of the waveguide as defined in Eq. (4), \( k = 2\pi/\lambda \) is the wave vector amplitude in vacuum. Eq. (8) is the equation of the Fourier components of Eq. (4).

When \( kL_p \ll 1 \), \( u(y) \) varies slowly at the \( L_p \) scale and \( u_q \approx 0 \) for \(|q| \neq 0 \). The effective medium result comes with the approximation that \( u(y) \approx u_0 \), which leads to the effective refractive as the zero frequency component of the effective refractive index profile: \( n_{TM} = \langle 1/n^2 \rangle^{-1/2} \) or \( \varepsilon_{TM} = \langle \varepsilon^{-1} \rangle \), where \( \langle \cdot \rangle \) means average value weighted by the layer thickness. Similarly for the TE mode the result is \( n_{TE} = \langle n^2 \rangle^{1/2} \) or \( \varepsilon_{TE} = \langle \varepsilon \rangle \).

This result is very similar with the well-known effective medium result for different polarizations \( \varepsilon_{\parallel} = \langle \varepsilon \rangle \) and \( \varepsilon_{\perp} = \langle \varepsilon^{-1} \rangle \) of a birefringent material, except that it is for the TE and TM modes, rather than for the electric field of different directions. It is worth noting that for the TM mode there are non-zero electrical field components in both parallel (z) and perpendicular (y) directions. This difference becomes noticeable when in the following we consider in more detail the anisotropic refractive index in a 1D waveguide, induced by the near-atomic-level layering of different semiconductor materials in the active region (material refractive index examples are shown in the insets in Fig. 2).

In Fig. 2 we compare the result of exact solution of Eq. (8) (by diagonalizing the linear operator on \( u_q \) in the left-hand-side up to a large enough cutoff) for the fundamental mode and the result of effective medium theory for two different periodic refractive index profiles, where we can see that: (a) for \( L_p \lesssim 0.1\lambda \) (where \( \lambda \) is the wavelength in vacuum) the effective medium theory is a very good approximation; (b) in the small wavelength limit \( (L_p/\lambda \to \infty) \), the result reduces to simple index guiding in the large refractive index region, so \( n_{eff} = n_{max} \); (c) if the effective refractive index were calculated from arithmetic averaging \( n_{eff} = \langle n \rangle \), it would lead to \( \lesssim 0.5\% \) error; considering relatively small refractive index contrast in many photonic structures, this can be non-negligible.
IV. GUIDED MODE CALCULATION WITH THE TRANSFER MATRIX METHOD

In QCLs as well as in conventional diode lasers, the waveguide claddings are typically implemented with several layers of different refractive index materials of sub-wavelength thickness. Such structure can be analytically solved using the transfer matrix method, as in Eq. (13)

Here we adopt the method for anisotropic materials (this can either be the layering-induced anisotropy discussed in the previous sections or material anisotropy), for the purpose of discussing the anisotropic gain/loss in QCLs. This is necessary because in the active region of a QCL, the gain is only on the electrical field in the y direction due to confined dipole direction, and the plasmonic loss is only in the x-z plane due to discrete quantum levels in y.

Eq. (4) can then be written as:

\[
\frac{n_y^2}{n_z^2} \frac{\partial}{\partial y} \frac{1}{n_z^2} \frac{\partial}{\partial y} H_x = -(n_y^2 - \beta^2) k^2 H_x \tag{9}
\]

The equation naturally suggests interface conditions by requiring \( H_x \) and \( (1/n_z^2) \partial H_x/\partial y \) to be continuous. This is consistent with the electrical field interface condition, which requires that \( D_y = \varepsilon_y \varepsilon_0 E_y = -H_x \beta k/\omega \) and \( E_z = \left[(1/n_z^2) \partial H_x/\partial y\right]/(i\omega \varepsilon_0) \) are continuous.

Within the same layer where \( n_{y,z} \) are constant,

\[
H_x(y) = H_x^+ e^{i\alpha y} + H_x^- e^{-i\alpha y} \tag{10}
\]

\[
E_z(y) = \gamma (H_x^+ e^{i\alpha y} - H_x^- e^{-i\alpha y}) \tag{11}
\]

\[
\gamma \equiv \frac{\alpha}{k n^2} \sqrt{\frac{\mu_0}{\varepsilon_0}} \tag{12}
\]

\[
\alpha \equiv k \sqrt{n_y^2 - \beta^2/n_y^2} \tag{13}
\]

where \( H_x^+ \) and \( H_x^- \) are the positive and negative y-propagating component of the magnetic field in x direction \( H_x \), \( \alpha \) is the y component of the effective wavevector, \( \gamma \) is the effective wave impedance.

The transfer matrix \( M_L \) for a layer with thickness \( L \) is given by:

\[
\begin{pmatrix}
E_z(0) \\
H_x(0)
\end{pmatrix} =
\begin{pmatrix}
\cos \alpha L & -i\gamma \sin \alpha L \\
-i\gamma^{-1} \sin \alpha L & \cos \alpha L
\end{pmatrix}
\begin{pmatrix}
E_z(L) \\
H_x(L)
\end{pmatrix} = M_L \begin{pmatrix}
E_z(L) \\
H_x(L)
\end{pmatrix} \tag{14}
\]

For complex valued \( \beta \) and \( n_{y,z} \), the square root in Eq. (13) is double-valued, but this does not affect the matrix \( M_L \) because all elements in the matrix are even functions of \( \alpha \). However, this double-value will affect the boundary condition for a guided mode, as we will show in the following.

Let the transfer matrix for \( i \)-th layer be \( M_i \). The transfer matrix for the whole structure is a matrix product of all \( M_i \)-s: \( M = \prod M_i = M_1 M_2 \cdots M_N \). For a guided mode the field decays before the first and after the last layer, which gives the boundary condition \( E_z(0^-) = -\gamma_0 H_x(0^-) \) and \( E_z(L^+) = \gamma_s H_x(L^+) \) by choosing only \( H_x^+ \) or \( H_x^- \) in Eq. (11). This means \( (\gamma_0, 1)^T \) is parallel to \( M(\gamma_s, 1)^T \), or:

\[
\chi_M(\beta) \equiv \gamma_s M_{11} + M_{12} + \gamma_s \gamma_0 M_{21} + \gamma_0 M_{22} = 0 \tag{15}
\]
where $\gamma_s$ and $\gamma_0$ are, respectively, the $\gamma$-s in Eq. (12) for the substrate after the last layer and for the environment before the first layer, and choosing the branch of the square root to have positive imaginary part $\Im \alpha > 0$; $M_{ij}$ is the $i$-th row, $j$-th column element of the matrix $M$. $\chi_M$ is called the modal-dispersion function. The modal-dispersion function transforms the eigen-problem Eq. (4) in function space to a root-finding problem.

The formula is applicable for both index guiding and for plasmonic guiding because the refractive index in the equations can be complex. For plasmonic guiding the only difference is that there should be a layer with real refractive index before the first layer, and choosing the branch of the square root to have positive imaginary part $\Im \gamma$. However, if we define a pseudo-inner product (pseudo because it is not positive definite) as:

$$\langle A_1, A_2 \rangle = \int \frac{1}{n_y^2} A_1 A_2 \, dy$$

the operator $\Theta$ is not Hermitian under the most commonly used inner product ($\langle A_1, A_2 \rangle = \int A_1 A_2 \, dy$) due to the position dependence of $n_y$ and due to the imaginary part of $n_y$ and $n_z$. However, if we define a pseudo-inner product (pseudo because it is not positive definite) as:

$$\langle A_1, A_2 \rangle = \int \frac{1}{n_y^2} A_1 A_2 \, dy$$

the operator $\Theta$ is Hermitian for a guided (modified from bounded) mode: $\langle A_1, \Theta A_2 \rangle = (\Theta A_1, A_2)$. With such an inner product, we can build a perturbation theory on $\Theta + \delta \Theta$:

$$\Rightarrow \delta \beta^2 = \frac{\langle H_x, \delta \Theta H_x \rangle}{\langle H_x, H_x \rangle}$$

when $\delta \Theta$ corresponds to a change in refractive index $\delta n$,

$$\langle H_x, H_x \rangle = \int \frac{1}{n_y^2} H_x^2 \, dy = \frac{\omega^2 c_0^2}{\beta^2} \int n_y^2 E_y^2 \, dy$$

$$\langle H_x, \delta \Theta H_x \rangle = \int H_x \left[ \frac{\delta n_y^2}{n_y^2} \frac{\partial}{\partial y} \frac{1}{n_z^2} \frac{\partial}{\partial y} + \frac{\partial}{\partial y} \frac{\delta n_z^2}{n_z^2} k^2 \right] H_x \, dy$$

$$= \int \delta n_y^2 \frac{H_x^2}{n_y^2} \, dy + \int H_y \frac{\partial}{\partial y} \frac{\delta n_z^2}{n_z^2} k^2 H_x \, dy$$

$$= \int \delta n_y^2 \left( \frac{\beta}{n_y^2} H_x \right)^2 \, dy - \int \frac{\partial}{\partial y} \frac{H_x^2}{n_z^2} \, dy$$

$$\omega^2 c_0 \left( \int n_y^2 E_y^2 \, dy + \int n_y^4 \frac{\delta n_z^2}{n_z^2} \, dy \right) \approx \omega^2 c_0 \int \delta n_y^2 E_y^2 \, dy$$

$$\delta \beta^2 \approx \frac{\int \delta n_y^2 E_y^2 \, dy}{\int n_y^2 E_y^2 \, dy} \frac{\delta n_z}{\Delta n_{\text{const. in AR}}} \Rightarrow \delta \beta \approx \frac{\beta}{\Delta n_z} \frac{n_z}{n_y^2} \frac{E_y^2}{E_y^2} \delta n_z \equiv \Gamma \delta n_z$$

where AR stands for the active region and as we will show, $\Gamma$ is the confinement factor when the non-
FIG. 3. The effective optical gain of the waveguide vs the imaginary susceptibility of the QC active material ((a) and (c)) and the relative error of the linear estimation ((b) and (d)), calculated from Eq. (28) and the confinement factor defined in Eq. (29)–(31). The non-perturbed result (dashed black line) from the transfer matrix method is considered the exact result. Insets are the waveguide structure for the calculation ((a) and (b); (c) and (d)): the blue lines and orange lines are the real and imaginary part of the refractive index respectively; green lines are the mode strength in arbitrary units, with the field in the active region colored red. In (a) and (c) the Eq. (28) and (29) curves are grouped because the difference is too small so that they overlap in the figure. A demonstration case where these two equations are noticeably different is shown in Fig. 4.

perturbed material is Hermitian.

This result is the optical version of the quantum mechanical treatment of Hamiltonian operators in Eq. (22).

For QCLs the change in the refractive index within the active region derives from the electrical dipoles between subbands, which is anisotropic \( \delta n_y = \chi \) the electrical susceptibility from the dipole moment and \( \delta n_z = 0 \), so the approximation in Eq. (24) becomes exact. For a generic gain medium the perturbation difference is not necessarily of this form, like in a diode laser, where the gain is often isotropic \( \delta n_y = \delta n_z \neq 0 \), this approximation is justified from the fact that \( E_z \) is usually much larger than \( E_x \) in a TM mode.

When we neglect the difference in group and phase velocities of the material, the gain of the medium is proportional to the imaginary part of the refractive index:

\[
I = I_0 \left| e^{i n \omega z / c} \right|^2 = I_0 e^{g z} \quad \Rightarrow \quad g = -2 \text{Im} \frac{\omega}{c} n \chi
\]

where \( I \) is the optical power flow and \( n \) is the complex refractive index, including the active gain. Similarly for a guided mode, \( g = -2 \text{Im} \frac{\omega}{c} \beta \). With \( n^2 = n_z^2 + \chi \) and \( \beta + \delta \beta \) given above, the relationship between the the active material gain (given in forms of \( \chi \)) and the waveguide effective gain \( g_{\text{eff}} \) induced by \( \chi \) is given by:

\[
\begin{align*}
g &= -2 \text{Im} \frac{\omega}{c} \sqrt{n_z^2 + \chi} \approx -\frac{\omega}{n_z c} \text{Im} \chi \quad \text{Eq. (27)} \\
g_{\text{eff}} &= -2 \text{Im} \frac{\omega}{c} \delta \beta = -\text{Im} \frac{\omega \beta_{\text{AR}}}{c} \int \chi E_z^2 \, dy \quad \text{Eq. (28)}
\end{align*}
\]

We employ a linear response form of \( g_{\text{eff}} = g \Gamma \) to define a confinement factor \( \Gamma \), but in general this is possible only
when the following are approximately true: (a) the gain medium is uniform on the wavelength scale and linear, i.e. \( \chi \) does not depend on the electrical field and is therefore constant for the active region; (b) the linear response does not mix the real and imaginary part of the perturbed refractive index, in other word, \( \Gamma \) in Eq. (25) is real.

In the simplest case where the material is low loss, the matrix in Eq. (14) means that the fields at different parts of the waveguide are always in phase, therefore, the confinement factor can be written in the following form that is more reminiscent to the frequently used formula

\[
\phi_{\text{eff}} = \Gamma g
\]

However, generally, the linear response of the waveguide effective gain for a perturbed bulk gain in the active region is not necessarily real, meaning \( \Gamma \) is complex or the real part of \( \chi \) has an effect on the imaginary part of \( \beta \) and vice versa. This becomes more relevant when the device is working on a frequency that’s off-resonance to the intrinsic frequency of the gain medium, where the Lorentzian shape introduces an out-of-phase component of the dipole oscillation and therefore an electrical susceptibility \( \chi \) with both non-zero real and imaginary part (versus, when working on-resonance, \( \chi \) is purely imaginary).

Comparing the above results and two frequently used formulas for the confinement factor:

\[
\Gamma_2 = \frac{\int_{\text{AR}} n|E|^2 \, dy}{\int |E|^2 \, dy}
\]

(30)

\[
\Gamma_3 = \frac{\int_{\text{AR}} |E|^2 \, dy}{\int |E|^2 \, dy}
\]

(31)

The difference is shown in Fig. 3 for the waveguide structure from (23) and (3) with different imaginary part of susceptibility in the active region, where we can see that the widely used confinement factor formulas have a few percent error compared to the revised version solution, while our equation shows one to two orders of magnitude smaller relative error, particularly the Eq. (28) is the exact linear term of the gain in active medium. It is worth mentioning that, in our context, the plasmonic boundary for the structure in Ref. (23) shares the same physical model as a double-metal waveguide for THz QCLs, except that the latter are more sensitive to the electrical and optical properties of the metal, which in turn depends on the metal deposition process and which we lack more information of; yet we are expecting our proposed formula to show similar improvement for double-metal waveguide.

To show when the difference between Eq. (28) and Eq. (29) is more significant, the comparison for a structure with alternating QC gain and high-doped lossy material is shown in Fig. 4. Such a structure may be of interest as a potential candidate for negative refractive index material.

VI. CONCLUSION

In summary, we have derived corrected formulas for the effective medium refractive index of the active region and the confinement factor for the purpose of QCL waveguide design. The difference to commonly used formulas of the confinement factor and effective refractive index in prior literature is up to a few percent in a typical waveguide for QCLs, due to the inaccurate linear response, due to neglecting the anisotropic property or the non-Hermitian property of the QC materials. The difference may become large when there is highly lossy material inside the device.

The method in this work can in straight forward manner be extended to other optical devices. By preserving the extra \( E_z \) term in Eq. (24) and by modifying the field vector basis in the transfer matrix Eq. (14) as in (11) the result can be easily generalized to any layered-structure active or passive optical devices for both TE and TM mode with isotropic or anisotropic gain.

ACKNOWLEDGMENTS

We would like to thank Yezhezi Zhang for helpful discussion with the potential application of this work to active meta-materials. This work was supported by the Intellectual Property Accelerator Fund received from Princeton University’s Office of the Dean for Research, and the Bede Liu Research Fund for Electrical Engineering received from Princeton University’s Department of Electrical and Computer Engineering.

DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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FIG. 4. The effective optical gain of the waveguide vs the imaginary susceptibility of the QC active material (left) and the relative error of the linear estimation (right), calculated from Eq. (28) and the confinement factor defined in Eq. (29)–(31). The non-perturbed result (dashed black line) from the transfer matrix method is considered the exact result. Insets are the waveguide structure for the calculation, where the blue lines and orange lines are the real and imaginary part of the refractive index respectively; green lines are the mode strength in arbitrary units, with the field in the active region colored red.

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