Coupled Wave Theory for Higher-Order Gratings

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1. Introduction

In this note, we present a detailed derivation of the modified coupled-mode equation for higher-order gratings. Using this equation, we demonstrate the existence of bound states in the continuum for second-order mirror-symmetric gratings.

2. Modified coupled mode equations

Following Ref. [1], we derive the modified coupled-mode equations for higher-order waveguide Bragg gratings. A quasi-TE mode in a waveguide grating of order N is governed by the Helmholtz equation:

$$\nabla^2 E_x(x,y,z) + k_0^2 n^2(x,y,z) E_x(x,y,z) = 0, \tag{1}$$

where $n(x,y,z)$ is the refractive-index profile, and $k_0 = 2\pi/\lambda$ is the vacuum wavenumber with λ being the wavelength in vacuum.
Since $n^2(x,y,z)$ is periodic in z for a waveguide grating extending along the z-axis, we may express it as a Fourier expansion:

$$n^2(x,y,z) = n_0^2(x,y) + \sum_{q\neq 0} A_q(x,y) \exp\left(j\frac{2\pi qz}{\Lambda}\right), \tag{2}$$

where Λ is the grating period, and $n_0^2(x,y)$ represents the relative permittivity profile averaged over one grating period.
Combining Eqs. 1 and 2, we obtain

$$\nabla^2 E_x + k_0^2 n_0^2 E_x + k_0^2 E_x \sum_{q\neq 0} A_q \exp\left(j\frac{2\pi qz}{\Lambda}\right) = 0, \tag{3}$$

where the summation index $q = \pm 1, \pm 2, \ldots$.
According to Bloch's theorem, the electric field of an eigenmode in a periodic medium can be expressed as an infinite series:

$$E_x(x,y,z) = \sum_{m=-\infty}^{\infty} E_x^{(m)}(x,y,z) \exp(j\beta_m z), \tag{4}$$

where $\beta_m = \beta_0 + \frac{2\pi m}{\Lambda}$, $\beta_0 = N\pi/\Lambda$ is the Bragg frequency, $E_x^{(m)}(x,y,z)$ represents the m-th order partial wave ($m = 0, \pm 1, \pm 2, \ldots$), which satisfies:

$$E_x^{(m)}(x,y,z) = E_{x,0}^{(m)}(x,y) \exp(j\delta z), \tag{5}$$

where $\delta = \beta - \beta_0 = \frac{2\pi n_{\text{eff}}}{\lambda} - \beta_0$ is the detuning of the propagation constant from the Bragg frequency.

Substituting Eq. 4 into Eq. 3 gives:

$$\nabla^2 \sum_{m=-\infty}^{\infty} E_x^{(m)}(x,y,z)\exp(j\beta_m z) + k_0^2 n_0^2 \sum_{m=-\infty}^{\infty} E_x^{(m)}(x,y,z)\exp(j\beta_m z)$$
$$+ k_0^2 \sum_{m=-\infty}^{\infty}\sum_{q\neq 0} A_q E_x^{(m)}(x,y,z)\exp\left[j\left(\beta_m + \frac{2\pi q}{\Lambda}\right)z\right] = 0.$$

For this equation to hold, the coefficient of each Fourier component must vanish.
Noting that all partial waves $E_x^{(m)}$ share the same oscillation frequency with respect to z (see Eq. 5), we obtain:

$$\nabla^2 E_x^{(m)}(x,y,z) + 2j\beta_m \frac{\partial}{\partial z}E_x^{(m)} + (k_0^2 n_0^2 - \beta_m^2)E_x^{(m)}(x,y,z) + k_0^2 \sum_{q\neq 0} A_q E_x^{(m-q)}(x,y,z) = 0. \quad (6)$$

This equation holds for all partial-wave orders $m = 0, \pm 1, \pm 2, \ldots$.
In particular, when $m = 0$ and the grating is weak ($|A_q| \ll 1$), Eq. 6 is approximately equivalent to the Helmholtz equation for the forward-propagating mode of a waveguide in the absence of a grating. Similarly, when $m = -N$ (for simplicity, denoted as $p = -N$), Eq. 6 can be interpreted as the equation governing the backward-propagating mode in the waveguide.

Therefore, we may write:

$$E_x^{(0)}(x,y,z) = R(z)E_0(x,y), E_x^{(p)}(x,y,z) = S(z)E_0(x,y), \quad (7)$$

where E_0 is the mode profile E_x of the unperturbed waveguide, while $R(z)$ and $S(z)$ are slowly varying functions of z representing the amplitudes of forward and backward waves, respectively.

Substituting Eq. 7 into Eq. 6 for $m = 0, p$ yields:

$$\nabla^2[R(z)E_0(x,y)] + 2j\beta_0 E_0(x,y)\frac{d}{dz}R(z) + (k_0^2 n_0^2 - \beta_0^2)R(z)E_0(x,y) + k_0^2 \sum_{q\neq 0} A_q E_x^{(-q)}(x,y,z) = 0, \quad (8.1)$$
$$\nabla^2[S(z)E_0(x,y)] + 2j\beta_p E_0(x,y)\frac{d}{dz}S(z) + \left(k_0^2 n_0^2 - \beta_p^2\right)S(z)E_0(x,y) + k_0^2 \sum_{q\neq 0} A_q E_x^{(p-q)}(x,y,z) = 0. \quad (8.2)$$

Note that E_0 satisfies the Helmholtz equation for a waveguide without a grating:

$$\frac{\partial^2}{\partial x^2}E_0 + \frac{\partial^2}{\partial y^2}E_0 + (k_0^2 n_0^2 - \beta^2)E_0 = 0, \quad (9)$$

where $\beta = \beta_0 + \delta$ is the propagation constant.

Combining Eqs. 8 & 9 and using $\beta_p = -\beta_0$, we obtain:

$$E_0 \frac{d^2}{dz^2} R + 2j\beta_0 E_0 \frac{d}{dz} R + (\beta^2 - \beta_0^2) R E_0 + k_0^2 \sum_{q \neq 0} A_q E_x^{(-q)} = 0, \tag{10.1}$$

$$E_0 \frac{d^2}{dz^2} S - 2j\beta_0 E_0 \frac{d}{dz} S + (\beta^2 - \beta_0^2) S E_0 + k_0^2 \sum_{q \neq 0} A_q E_x^{(p-q)} = 0. \tag{10.2}$$

When considering modes near the Bragg frequency, $R(z)$ and $S(z)$ are slowly varying functions of z. Hence, the terms proportional to d^2R/dz^2 and d^2S/dz^2 can be neglected, resulting in:

$$2j\beta_0 \frac{dR}{dz} E_0 + (\beta^2 - \beta_0^2) R E_0 + k_0^2 A_{-p} S E_0 + k_0^2 \sum_{q \neq 0, -p} A_q E_x^{(-q)} = 0, \tag{11.1}$$

$$-2j\beta_0 \frac{dS}{dz} E_0 + (\beta^2 - \beta_0^2) S E_0 + k_0^2 A_p R E_0 + k_0^2 \sum_{q \neq 0, p} A_q E_x^{(p-q)} = 0. \tag{11.2}$$

Multiplying both sides of Eq. 11 by E_0^* and integrating over the waveguide cross-section yields:

$$\frac{dR}{dz} - j\delta R - j\kappa_p^* S - \frac{jk_0^2}{2\beta_0 P} \sum_{q \neq 0, -p} \int A_q E_0^* E_x^{(-q)} dxdy = 0, \tag{12.1}$$

$$-\frac{dS}{dz} - j\delta S - j\kappa_p R - \frac{jk_0^2}{2\beta_0 P} \sum_{q \neq 0, p} \int A_q E_0^* E_x^{(p-q)} dxdy = 0, \tag{12.2}$$

where we have used the approximation $\beta^2 - \beta_0^2 \approx 2\beta_0 \delta$. The parameters P, κ_p, κ_p^* are defined as:

$$P = \int |E_0|^2 dxdy, \tag{13.1}$$

$$\kappa_p = \frac{k_0^2}{2\beta_0 P} \int A_p |E_0|^2 dxdy, \tag{13.2}$$

$$\kappa_{-p} = \frac{k_0^2}{2\beta_0 P} \int A_{-p} |E_0|^2 dxdy = \kappa_p^*. \tag{13.3}$$

Note that ***P* represents the integrated optical intensity, not the optical power.**

To solve Eq. 12, we need to evaluate the partial waves $E_x^{(m)}$ of different orders $(m \neq 0, p)$ using Eq. 6. To simplify the formulation, we neglect the $\partial E_x^{(m)}/\partial z$ term and assume that $E_x^{(0)}, E_x^{(p)}$ dominate the series expansion. These approximations are valid when the detuning from the Bragg frequency is small and the grating is weak. Under these assumptions, and combining Eqs. 6 & 7, we have:

$$\nabla^2 E_x^{(m)} + (k_0^2 n_0^2 - \beta_m^2) E_x^{(m)} = -k_0^2 E_0 \left(A_m R + A_{m-p} S\right), m \neq 0, p. \tag{14}$$

The solution to this equation takes the form:

$$E_x^{(m)} = RE_m^{(0)} + SE_m^{(p)}, \tag{15}$$

where E_m^0 and $E_m^{(p)}$ satisfy:

$$\nabla^2 E_m^{(i)} + (k_0^2 n_0^2 - \beta_m^2) E_m^{(i)} = -k_0^2 A_{m-i} E_0, m \neq 0, p; i = 0, p. \tag{16}$$

Substituting Eq. 15 into Eq. 12 yields the **modified coupled-mode equations** for the higher-order grating:

$$\frac{dR}{dz} - j(\delta + \zeta_1)R = j(\kappa_p^* + \zeta_2)S, \tag{17.1}$$

$$-\frac{dS}{dz} - j(\delta + \zeta_3)S = j(\kappa_p + \zeta_4)R, \tag{17.2}$$

where ζ_{1-4} are **Streifer terms** (first introduced by William Strifer in [2]) defined as:

$$\zeta_1 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, -p} \int A_q E_0^* E_{-q}^{(0)} dxdy,$$

$$\zeta_2 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, -p} \int A_q E_0^* E_{-q}^{(p)} dxdy,$$

$$\zeta_3 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, p} \int A_q E_0^* E_{p-q}^{(p)} dxdy,$$

$$\zeta_4 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, p} \int A_q E_0^* E_{p-q}^{(0)} dxdy.$$

Here, the terms $E_m^{(i)}$ are obtained by solving Eq. 16. The definitions of P and κ_p are given in Eq. 13.

3. Dispersion relation for symmetric waveguide grating

In all cases, $\zeta_1 = \zeta_3$; when the grating is mirror-symmetric, that is, when $n^2(x, y, z)$ is an even function of z, we also have $\zeta_2 = \zeta_4$. Below, we restrict our discussion to this specific case. In this case, both A_p and κ_p are real. Combining Eqs. 17.1 and 17.2, we obtain:

$$\left[(\delta + \zeta_1)^2 - (\kappa_p + \zeta_2)^2 + \frac{d^2}{dz^2}\right] R = 0.$$

To solve for the mode eigenfrequency in the grating, we use substitutions $\delta \to \frac{\Delta\omega}{v_g}, \frac{d^2}{dz^2} \to -k^2$, which yield:

$$\frac{\Delta\omega}{v_g} = -\zeta_1 \pm \sqrt{\left(\kappa_p + \zeta_2\right)^2 + k^2}, \tag{18}$$

where $\Delta\omega$ is the eigenfrequency detuning from $\frac{c\beta_0}{n_{\text{eff}}}$, v_g is the group velocity of the waveguide (in the absence of the grating), $k = \beta - \beta_0$ is the Bragg wave-vector detuning from the Bragg frequency β_0.

4. Bound state in the continuum

Moreover, when the grating is 2nd-order and mirror-symmetric, it can be shown that the imaginary parts of ζ_1, ζ_2 are equal [3] (a proof is provided below). Therefore, for the two branches of eigenmodes described by Eq. 18, one branch exhibits zero radiation loss (recalling that κ_p is real) at $k = 0$, while the other exhibits enhanced radiation loss. The eigenmode with suppressed radiation loss is known as a bound state in the continuum (BIC).

Existence theorem for BIC

For a 2nd-order mirror-symmetric grating ($p = -2$, $n^2(x, y, -z) = n^2(x, y, z)$), there exists an eigenmode at the Bragg frequency with zero radiation loss.

Proof

To prove the existence of a BIC in a 2nd-order mirror-symmetric grating, it suffices to show that $\text{Im}(\zeta_1) = \text{Im}(\zeta_2)$. The existence of the BIC then follows from Eq. 18 (noting again that κ_p is real).

When no grating is present, the waveguide is lossless, and E_0 can be chosen to be real through an appropriate choice of phase reference [4].

As stated previously, ζ_1, ζ_2 are given by:

$$\zeta_1 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, -p} \int A_q E_0^* E_{-q}^{(0)} dxdy, \tag{19.1}$$

$$\zeta_2 = \frac{k_0^2}{2\beta_0 P} \sum_{q \neq 0, -p} \int A_q E_0^* E_{-q}^{(p)} dxdy, \tag{19.2}$$

where $E_m^{(i)}$ is determined from Eq. 16:

$$\nabla^2 E_m^{(i)} + (k_0^2 n_0^2 - \beta_m^2) E_m^{(i)} = -k_0^2 A_{m-i} E_0, m \neq 0, p; i = 0, p. \tag{20}$$

Eq. 20 is an inhomogeneous Helmholtz equation of the form $\nabla^2 A + k^2 A = -f$ with $k_m^2 = k_0^2 n_0^2 - \beta_m^2$ and $f = k_0^2 A_{m-i} E_0$. Assuming the spatial variation of the refractive index is weak such that $k_0^2 n_0^2 \approx k_0^2 n_{\text{eff}}^2$, we obtain:

$$k_m^2 = k_0^2 n_{\text{eff}}^2 - \beta_m^2 = (\beta_0 + \delta)^2 - \left(\beta_0 + \frac{2\pi m}{\Lambda}\right)^2 = \left(\frac{\pi N}{\Lambda} + \delta\right)^2 - \left(\frac{\pi N}{\Lambda} + \frac{2\pi m}{\Lambda}\right)^2, \tag{21}$$

where the grating order $N = 2$, the detuning δ is assumed to be small, and m is an integer representing the partial-wave order. For a 2nd-order grating, $k_m^2 < 0$ only when $m = -1$, otherwise $k_m^2 > 0$.

Recalling that the solution to Eq. 20 can be expressed as an integral over the Green's function [5]:

$$E_m^{(i)} = \int k_0^2 A_{m-i}(\boldsymbol{r}')E_0(\boldsymbol{r}')G_m(\boldsymbol{r},\boldsymbol{r}')d\boldsymbol{r}' , \tag{22.1}$$

$$G_m(\boldsymbol{r},\boldsymbol{r}') = \frac{\exp(jk_m|\boldsymbol{r}-\boldsymbol{r}'|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{22.2}$$

where both $\boldsymbol{r}$ and $\boldsymbol{r}'$ are two-dimensional position vectors: $\boldsymbol{r} = (x, y)$, $\boldsymbol{r}' = (x', y')$.

Combining Eqs. 21 and 22, and recalling that E_0 is real (due to lossless waveguide) and that A_{m-i} is real for a mirror-symmetric grating, we find that:

When $m = -1$, k_m is an imaginary number, $E_m^{(i)}$ possesses a nonzero imaginary part.
Otherwise $E_m^{(i)}$ is a real-valued field.

From this observation and Eq. 19, the imaginary parts of ζ_1, ζ_2 reduce to:

$$\mathrm{Im}(\zeta_1) = \frac{k_0^2}{2\beta_0 P}\mathrm{Im}\left[\iint A_1 E_0^* E_{-1}^{(0)} dxdy\right], \tag{23.1}$$

$$\mathrm{Im}(\zeta_2) = \frac{k_0^2}{2\beta_0 P}\mathrm{Im}\left[\iint A_1 E_0^* E_{-1}^{(-2)} dxdy\right]. \tag{23.2}$$

Since $A_1 = A_{-1}$ for a mirror-symmetric grating, it follows from Eq. 22 that $E_{-1}^{(0)} = E_{-1}^{(-2)}$. Therefore, we conclude that:

$$\mathrm{Im}(\zeta_1) = \mathrm{Im}(\zeta_2). \tag{24}$$

This relationship proves the **existence of a bound state in the continuum (BIC).**

Q.E.D.

Reference

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