Coupled Mode Theory of Optomechanical Crystals

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Abstract—Acousto-optic interaction in optomechanical crystals allows unidirectional control of elastic waves over optical waves. However, as a result of this nonlinear interaction, infinitely many optical modes are born. This article presents an exact formulation of coupled mode theory for interaction between elastic and photonic Bloch waves moving along an optomechanical waveguide. In general, an optical wavefront is strongly diffractioned by an elastic wave in frequency and wavevector, and thus infinite modes with different frequencies and wavevectors appear. We discuss resonance and mode conversion conditions, and present a rigorous method to derive coupling rates and mode profiles. We also find a conservation law which rules over total optical power from interacting individual modes. We present application examples to the theory to optomechanical waveguides and cavities, as well as non-reciprocal transmission of light and optomechanical switches.

Index Terms—Photonic Crystals, Phononic Crystals, Optomechanics, Optical MEMS

I. INTRODUCTION

An optomechanical crystal is essentially a periodic photonic crystal [1] in which electromagnetic waves may propagate at certain frequencies and directions, while mechanical elastic waves are also launched simultaneously. The mechanical waves obey the elastic Bloch properties of the same medium being treated as a periodic phononic crystal. The photo-elastic interaction [2], [3], [4] between an elastic wave with frequency \( \omega \) and electromagnetic wave at a much higher frequency \( \omega \) leads to a type of nonlinear phenomenon which produces new harmonics as \( \omega \pm \Omega \). While both types of waves propagate in the same type of periodic medium, and observe similar Bloch-periodicity and orthogonality conditions [5], their existence are connected through the photo-elastic tensor [2], [4] which contributes through the constitutive relations for electric field and displacement vectors.

In piezo-electric media, low frequency electromagnetic waves may strongly couple and co-exist with their elastic waves, giving rise to a different type of piezo waves, and hence \( \omega = \Omega \). Such linear waves may also observe Bloch-periodicity in periodic background, and generate a bandstructure [6] exhibiting wide bandgaps. This is different from the scope of this paper in which optical and elastic waves interact nonlinearly.

This field was brought to the attention by a landmark paper in 2003 [7], which reported strong Doppler shifting of reflecting electromagnetic waves from an acoustic shock wave. This rapidly opened up numerous applications in the area of phononic crystals [8], while the recent applications of optomechanics has gone well beyond of classical regime, and quantum mechanical phenomena are being studied. These include manipulation of photo-luminescence [9], spin control in diamond Nitrogen vacancies for quantum computing purposes [10], tuning photonic crystals with phonons [11], and coherent wavelength conversion [12]. Current literature in this area is now quite vast, which is reviewed in several extensive works [13], [14].

The main difficulty with the numerical study of this area arises from the many orders of magnitude difference between the optical \( \omega \) and acoustic \( \Omega \) frequencies, which is typically being on order of \( 10^6 \) to \( 10^7 \). Hence, time-domain methods such as nonlinear Finite-Difference Time-Domain [15], [16] developed for second-order and third-order nonlinear interactions are essentially inefficient to reproduce useful results. The reason is that the total computational time should be at least of the order of \( 10^3 \) to \( 10^4 \) acoustic time-cycles, which considering the very tiny time-steps being required for ultrashort optical cycles, demands a very huge number of total time steps. For a typical simulation this number of total time-steps could easily blow up to anywhere from \( 10^{10} \) to \( 10^{12} \), or even more. This is well beyond the capability of a general purpose personal computer, unless the elastic wave is supposed to be frozen at relatively large time intervals. This method has been implemented by some authors [17], [18], but is unable to take care of the frequency differences of Doppler shifts caused by the acousto-optic interaction.

It had been assumed that mechanical loss is a major obstacle to propagate elastic waves inside phononic waveguides over long distances, however, with the recent progress in understanding of propagation of mixed bulk-surface elastic waves [19], hope for near-lossless propagation in slabs has come into the light. Interestingly, for all practical purposes, two-dimensional slabs of periodic media are being widely studied [20] since true three-dimensional structures cannot exist. Examples include optomechanical interactions in thin membranes such as single-layer graphene [21], [22], [23], [24] and ultrathin high-stress Si\(_3\)N\(_4\) membranes [25], [26]. Recent progress in fabrication of ultrathin Si\(_3\)N\(_4\) membranes [25], [26] has resulted in record long-lived confined modes, reaching room-temperature quality factors in excess of \( 10^8 \) at \( \Omega = 1\)MHz [27]. This remarkable achievement has demonstrated the possibilities for strong photon-phonon interactions over large time intervals, even at elevated temperatures. Enhanced scattering in the subwavelength regime in Si nanostructures is being also shown and pursued [28].

It is the purpose of this paper to develop a full and exact theoretical understanding of the nonlinear interaction between elastic and electromagnetic waves from a classical point of
view. Without loss of generality, we assume simple dielectric, that is being nonmagnetic, linear, isotropic, and lossless. Using a harmonic-balance method we identify and equate various harmonics propagating at different frequencies and directions. We obtain a set of coupled-mode equations, comparable to those known in standard coupled-mode theory \[2\], \[3\], \[4\], which may be solved accurately at discretion, obtaining coupling rates or coupling lengths. Our results confirm the earlier findings \[32\] based on the boundary perturbation theory \[33\]. We also present an application example to non-reciprocal transmission of light inside an optomechanical waveguide.

## II. Theory

The photo-elastic interaction is described using the equation \[2\], \[3\], \[4\]

$$
\Delta \eta_{ij} = p_{ijmn} S_{mn}, \quad T_{mn,n} = (c_{mnij} S_{ij}),_n = -\Omega^2 \rho u_i,
$$

where \(p_{ijmn}\) are the elements of the fourth-rank photo-elastic tensor, \(\eta_{ij}\) are elements of the impermeability tensor, and \(S_{mn} = \frac{1}{2}(u_{mn} + u_{nm})\) are strain components obtained from the displacement vector field \(u\). Furthermore, \(\rho, T_{mn}\) and \(c_{mnij}\) are respectively the mass density, and the elements of the stress and stiffness tensor. Symmetry considerations \[4\] require that \(p_{ijmn} = p_{jimn} = p_{ijmn}\) to maintain \(S_{mn} = S_{nm}\) and \(\eta_{ij} = \eta_{ji}\).

We here adopt a dimensionless system of variables for Maxwell’s equations, where \(\epsilon_0\) and \(\mu_0\) are dropped and the light velocity \(c = 1\) is normalized. Furthermore, the lattice constant \(a\) of the periodic medium is set to unity and all frequency and length measures are correspondingly normalized. Since the medium is taken to be simple, then unperturbed permittivity tensor is simply \(|\epsilon| = \epsilon(r)|l|\), where \(\epsilon(r) = n^2(r)\) is the position-dependent squared refractive index. Evidently, this is going to be a biperiodic function of position as \(\epsilon(r) = \epsilon(r + R)\) with \(R\) being any discrete lattice vector.

The change in the permittivity of bulk due to a strain field is thus

$$
\Delta \epsilon = (\epsilon^{-1}|l| + [\Delta \eta])^{-1} - \epsilon|l|.
$$

If the perturbation is sufficiently small, then \[2\] may be approximated as

$$
\Delta \epsilon \approx -[\epsilon]|[\Delta \eta]|\epsilon = -\epsilon^2 [\Delta \eta],
$$

or

$$
\Delta \epsilon_{ij} \approx -\epsilon a pt_{kijm} S_{mn} \epsilon_{kj} = -\epsilon^2 p_{ijmn} S_{mn}.
$$

The strain field \([S] = [S(r, t)]\) is actually a function of position and time, corresponding to a moving elastic wave at frequency \(\Omega\), and therefore \([\Delta \epsilon] = [\Delta \epsilon(r, t)]\). It is here appropriate to decompose \([\Delta \epsilon]\) as

$$
[\Delta \epsilon] = \frac{1}{2} [\delta \epsilon](e^{j\Omega t} + e^{-j\Omega t}),
$$
in which \([\delta \epsilon]\) is a time-independent, but position-dependent symmetric real tensor.

We may now proceed with the Maxwell’s equations

\[
\nabla \times \vec{E}(r, t) = -\frac{\partial}{\partial t} \vec{H}(r, t),
\]

\[
\nabla \times \vec{H}(r, t) = +\frac{\partial}{\partial t} \vec{D}(r, t),
\]

where \(\vec{D} = [\epsilon] \vec{E}\). Plugging \[5\] in \[6\], \[7\] and some algebraic simplification gives the coupled set of balanced harmonic equations for the complex phasor vector fields \((\vec{E}_n, \vec{H}_n)\), being here referred to as modes, at the frequency component \(\omega_n = \omega + n\Omega\) as

$$
\nabla \times \vec{E}_n(r) = -i\omega_n \vec{H}_n(r)
$$

$$
\nabla \times \vec{H}_n(r) = +i\omega_n \vec{D}_n(r)
$$

in which the displacement field of the harmonic \(n\) is given by

$$
\vec{D}_n = \epsilon \vec{E}_n + \frac{1}{2} [\delta \epsilon](\vec{E}_{n+1} + \vec{E}_{n-1}),
$$

with the dependence on position vector \(r\) dropped for convenience.

It is here furthermore understood that the modes are not true- or spatial-harmonics of the same frequency as opposed to the theory of nonlinear optics \[2\], diffraction theory of gratings \[29\], or multi-port networks \[30\], \[31\], since in general \(\Omega\) is not an integer divisor of \(\omega\). The total fields may be now recovered from the summation over individual modes as

$$
\vec{E}(r, t) = \sum_n \Re[\vec{E}_n(r)e^{i\omega_n t}],
$$

$$
\vec{H}(r, t) = \sum_n \Re[\vec{H}_n(r)e^{i\omega_n t}].
$$

These constitute the total incident and scattered optical fields due to the nonlinear mixing of optical and elastic waves at the original frequencies \(\omega\) and \(\Omega\), respectively.

### A. Coupling coefficients

It is possible to make use of the vector identity \(A \cdot \nabla \times B = B \cdot \nabla \times A - \nabla \cdot (A \times B)\), multiplying \[6\] and \[7\], respectively with \(\vec{H}_n^*\) and \(\vec{E}_n^*\), and subtracting to obtain the master power equation

$$
\nabla \cdot \vec{S}_n = \omega_n \Im[\vec{U}_{en} + \vec{U}_{mn}],
$$

Here, \(\vec{S}_n = \frac{1}{2} \Re[\vec{E}_n \times \vec{H}_n^*]\) is the time-averaged Poynting’s vector, and \(\vec{U}_{en} = \frac{1}{2} \epsilon \vec{E}_n \cdot \vec{D}_n\) and \(\vec{U}_{mn} = \frac{1}{2} \vec{H}_n \cdot \vec{H}_n\) are respectively the time-averaged electric and magnetic energy densities of the \(n\)th harmonic. Integration of \[13\] over the crystal’s unit cell will give rise to the coupling coefficients due to the photoelastic, or the so-called bulk electrostrictive forces \[34\] as demonstrated below.

One may view the sharp boundaries across dielectrics be softened by a gradual variation of mass density and stiffness within a given virtual transition thickness \(t\), while assuming
where the case of effect of radiation pressure into account [32] and ignoring the electrostriction as a unit cell to obtain and is here denoted by UC. Now, (13) may be integrated over a unit cell to obtain

\[ I_n(1) - I_n(0) = \omega_n \int_{UC} \Re[U_{en} + U_{mn}] d^2r, \quad (14) \]

where \( I_n(x) \) denotes the total optical power of the \( n \)th harmonic propagating along the direction +\( x \). Expansion of the integrand here using (10) gives

\[ \Re[U_{en} + U_{mn}] = \frac{1}{2} \Re\left[ E_n^* \cdot [\delta \epsilon](E_{n+1} + E_{n-1}) \right], \quad (15) \]

since \( \Re[H_n^*H_n] = 0 \), and also \( \Re[E_n^*\cdot[\epsilon]E_n] = 0 \) by transpose symmetry of \( [\epsilon] \). This will simplify (13) as

\[ I_n(1) - I_n(0) = \frac{\omega_n}{2} \Re\int_{UC} E_n^* \cdot [\delta \epsilon](E_{n+1} + E_{n-1}) d^2r. \quad (16) \]

We may now define the coupling rate \( \alpha_n \) and coupling length \( L_n = \alpha_n^{-1} \) as \( I_n(1) = I_n(0)e^{-\alpha_n} \). Hence, if we have normalized the \( n \)th harmonic power as \( I_n(0) = 1 \), then for the case of \( L_n \gg 1 \) we have

\[ \alpha_n \approx -\frac{\omega_n}{2} \Re\int_{UC} E_n^* \cdot [\delta \epsilon](E_{n+1} + E_{n-1}) d^2r, \quad (17) \]

subject to the normalization

\[ I_n(0) = \int_{-\infty}^{+\infty} S_n \cdot \hat{x} dy = 1, \quad (18) \]

for all \( n \). The result (17) may be compared to the expression which can be constructed in a similar way by only taking the effect of radiation pressure into account [32] and ignoring the electrostriction as (18) still applies. In general, one needs to add up the effect of both these two terms (18) and (19) in order to obtain the correct answer [17], however, as discussed in the previous section, usually one effect may dominate [34], under the above mentioned conditions.

### B. Conservation law

Interestingly, a conservation law for total optical power may be found by summing up (16) over all harmonics as

\[ I(1) - I(0) = \Omega \int_{-\infty}^{\infty} \Re\int_{UC} E_{n+1}^* \cdot [\delta \epsilon]E_n d^2r, \quad (20) \]

The right-hand-side of (20) is proportional to frequency of elastic waves \( \Omega \), and depending on its sign describes the total power withdrawn from or deposited into the acoustic wavefront during the process of nonlinear mixing with optical beam. This result also makes use of the supposed lossless property of the dielectrics, which comes as the real symmetry of the tensor \( [\delta \epsilon] \). In practice, we have \( \Omega \) being much smaller than \( \omega \) by five to six orders of magnitude, hence, in other words to a very reasonable approximation, the total optical power is a conserved quantity while it is divided and continuously being exchanged among various harmonics according to

\[ I(1) - I(0) \approx 0. \quad (21) \]

### C. Resonance conditions

1) **Optomechanical waveguides:** In the infinitely-many coupled-mode equations (16), only a few in practice dominate which satisfy the condition of resonant power exchange. All other modes out of resonance will be return the fetched power from other modes soon after propagation a few lattice constants along the waveguide. The reason becomes obvious by expansion of Bloch eigenmodes [5] as

\[ E_n(r; \kappa_n) = e^{-i\kappa_n x} e(r; \kappa_n) = e^{-i\kappa_n x} \sum_{G} e_{\kappa_n}(y; G) e^{-iGx}, \quad (22) \]

in which \( \kappa_n \) is the Bloch wavevector, \( G = G_m = 2\pi m \) are reciprocal lattice vectors, and \( e(r; \kappa_n) = e(r + \hat{x}; \kappa_n) \) is the periodic envelope function of the \( n \)th harmonic. Similarly, we may use

\[ [\delta \epsilon(r)] = \Re[e^{-ikx}[\theta](r; k)], \quad (23) \]

with \( k \) and \( [\theta](r; k) \) respectively being the Bloch wavevector and envelope of the permittivity tensor, as a result of moving elastic wave.

Insertion of (22) and (23) in (17) gives

\[ \alpha_n \approx -\frac{\omega_n}{4} \Re\int_{UC} d^2r \sum_{G,G',G''} (S_1 + S_2 + S_3 + S_4), \quad (24) \]
where the expressions for $S_1$, $S_2$, $S_3$, and $S_4$ are given by

$$S_1 = e^{i[(\kappa_n - \kappa_{n-1}) - k + G - G' - G'']x} \times \mathbf{e}_{\kappa_n}(y; G) \cdot [\theta]_{nk}(y; G') \mathbf{e}_{\kappa_{n-1}}(y; G''),$$
$$S_2 = e^{i[(\kappa_n - \kappa_{n+1}) + k + G - G' - G'']x} \times \mathbf{e}_{\kappa_n}(y; G) \cdot [\theta]_{nk}(y; G') \mathbf{e}_{\kappa_{n+1}}(y; G''),$$
$$S_3 = e^{i[(\kappa_n - \kappa_{n-1}) + k + G + G' - G'']x} \times \mathbf{e}_{\kappa_n}(y; G) \cdot [\theta]_{nk}^*(y; G') \mathbf{e}_{\kappa_{n-1}}(y; G''),$$
$$S_4 = e^{i[(\kappa_n - \kappa_{n+1}) - k + G + G' - G'']x} \times \mathbf{e}_{\kappa_n}(y; G) \cdot [\theta]_{nk}^*(y; G') \mathbf{e}_{\kappa_{n+1}}(y; G'').$$

The coupled-mode equations can be further simplified for resonant modes which satisfy the momentum equation $\kappa_n - \kappa_{n-1} \pm k = 2\pi l$ where $l$ is an integer. In that case, only one of the above integrals does not vanish while integrating along many unit cells, and the other three will decay to zero. Practically, the surviving modes will be limited only to $n = 0$ and one of the harmonics $n = \pm 1$ since it would be normally impossible to satisfy all resonant criteria at once for all other harmonics.

Let us take $S_4$ as the resonant non-vanishing term, in which the initial wave at $n = 0$ with frequency $\omega$ and the elastic wave with frequency $\Omega$ propagate in the same direction and the up-converted optical mode with $n = 1$ and frequency $\omega_1 = \omega + \Omega$ is counter-propagating. Hence, the counter-propagating up-converted optical beam must have opposing symmetry to the initial input beam. This can be satisfied only if the corresponding symmetries to the $n = 0$ optical wave and elastic wave are different, in such a way that the integral in (24) over the transverse direction $y$ does not vanish.

This condition may be easily satisfied in dielectric photonic crystal waveguides made out of two-dimensional triangular lattice, by simply removing one row of air holes along the $\Gamma\text{M}$ direction, where both even and odd branches co-exist within the same frequency range across the photonic bandgap.

For this purpose, the recently proposed snow-flake optomechanical crystals [33] with some modifications could possibly provide a natural basis background lattice if simply one row of air defects are removed. The snow-flake optomechanical crystals exhibit the remarkable property of having both full mechanical and H-polarized optical bandgaps. Of course, one may need to carefully engineer the resulting waveguide to make sure about the existence of crossing even-odd guided optical branches as well as at least one even or odd mechanical branch. Another interesting option is the very recent triangular design of patterned membranes [27] which exhibit an outstanding near-lossless operation and prolonged mechanical lifetimes.

The relation (23) will then simplify as

$$\alpha_n \approx -\frac{2\pi \omega_n}{4} \int \frac{dy}{\infty} \sum_{G, G'} \mathbf{e}_{n'}^*(y; G) \cdot [\theta]_{nk}^*(y; G') \mathbf{e}_{n-1}(y; G''),$$

where we note that $G$, $G'$, and $G''$ are not all independent at once, satisfying $G + G' - G'' = 2\pi l$ for some $l$. This would clearly correspond to the Umklapp process [36], which folds back the scattered waves with wavevectors outside the first Brillouin zone unto the equivalent waves inside the first Brillouin zone.

Hence, there are four different resonance conditions which need to be satisfied at one to obtain a strong interaction between elastic and optical waves:

1) Conservation of photon-phonon energies $\hbar \omega_n = \hbar \omega + nh\Omega$.
2) Conservation of momentum $\kappa_n - \kappa_{n+1} \pm k = 2\pi l$ is a reciprocal lattice vector.
3) Matching transverse symmetry, that is all of the three initial and scattered optical wave and elastic wave are even, or exactly two out of these are odd.
4) Matching polarization, so that the perturbation permittivity $[\delta e]$ caused by the elastic field, would be sensed both by the initial and scattered optical waves.

Consideration of these four requirements, reveals that it is not possible to have both the initial and scattered optical modes on the same waveguiding dispersion curve. Instead, they may have opposite transverse symmetries and very close frequencies differing only by $\Omega$. For this purpose, the photonic crystal waveguide must have the two even and odd branches present and crossing at once, as discussed in the above.

This could be now easily exploited to design a non-reciprocal photonic crystal waveguide discussed in the above, where an odd acoustic wave is propagating in background along a preferred direction. Now, any incoming optical wave with even symmetry would be scattered into an odd mode, and of course with a tiny amount of shift in frequency. However, the same scattering could not be reversed in direction. If the even optical wave is coming from the opposite direction, scattering unto an odd wave would be impossible. Hence, the scattering criteria for waves coming from both directions could not be met at once. This is exactly the non-reciprocal operation.

There is an extra advantage of this design over other designs. First of all, the Umklapp process could be exploited to design many essentially different scatterings, such as optical even to even through mechanical even, optical even to odd through mechanical odd, optical odd to odd through mechanical even, and as such, which go beyond the first Brillouin zone. Secondly, an optically guided Gaussian pulse with relatively wide spectrum in frequency and wavenumber could be completely scattered in whole, to another Guassian pulse. Equivalently, the phase matching criteria are not so restrictive, as fabrication imperfections as well as some spread in the acoustic spectrum would allow some degree of fuzziness over the mathematically accurate expressions.

2) Optomechanical cavities: In the case of optomechanical cavities, where no propagation occurs for any type of the waves, the momentum condition in the above is irrelevant and may be dismissed. Here, the energy exchange between optical modes will cause appearance of a small imaginary part in the frequencies as $\omega_n = \omega_n + i\beta_n$, where $\beta_n$ represents the power
loss or intake rate for the $n$th mode. The master equation (13) may be modified now as

$$\nabla \cdot \mathbf{S}_n = 3[\tilde{\omega}_n(U_{en} + U_{mn})].$$  (26)

and then integrated over the entire $x-y$ plane to obtain

$$\int \int 3[\tilde{\omega}_n(U_{en} + U_{mn})] d^2 r = 0.$$  (27)

Separation of real and imaginary parts now gives

$$\frac{\beta_n}{\omega_n} = -\frac{\int \int 3|U_{en} + U_{mn}| d^2 r}{2 \int \int 3|U_{en} + U_{mn}| d^2 r}.$$  (28)

Now, plugging in (15) gives

$$\beta_n = -\frac{\omega_n}{2} \int \int \left|E_n^* \cdot \delta \varepsilon (E_{n+1} + E_{n-1}) \right| d^2 r.$$  (29)

for the rate $\beta_n$. Hence, the typical time-constant at which the energy is exchanged with the $n$th mode of the cavity is $\tau_n = \beta_n^{-1}$. It has to be noticed that while evaluating (29), that it is subject to the normalization condition for electromagnetic energy of individual modes, equating the denominator to unity for all modes. Hence, we get

$$\beta_n = -\frac{\omega_n}{2} \int \int \left|\mathbf{E}_n^* \cdot \delta \varepsilon (\mathbf{E}_{n+1} + \mathbf{E}_{n-1}) \right| d^2 r.$$  (30)

Again, apart from the requirements for conservation of photophonon energies, symmetry of modes, and matching polarizations, not every photonic cavity allows co-existence of two energy levels, symmetry of modes, and matching polarizability equations between a time-harmonic elastic field, for individual harmonics, which because of strict resonance conditions would be practically limited to very few surviving modes. Expressions for the coupling rates and lengths were obtained in case of optomechanical waveguides. A conservation law was obtained which satisfied the preservation of total optical power and withdrawn power from the elastic field, however, it was discussed that the contribution from the latter part may be negligible when the frequencies of these two fields differ by many orders of magnitude, hence preserving the total optical power. We also discussed the extension of this theory for using in analysis of optomechanical cavities. Application examples to non-reciprocal light transmission inside an optomechanical waveguide, and also conceptual design of optomechanical switches were discussed.

III. CONCLUSIONS

We presented a rigorous approach to solve the optomechanical coupling equations between a time-harmonic elastic field and an optical field. An infinite set of equations were resulted for individual harmonics, which because of strict resonance conditions would be practically limited to very few surviving modes. Expressions for the coupling rates and lengths were obtained in case of optomechanical waveguides. A conservation law was obtained which satisfied the preservation of total optical power and withdrawn power from the elastic field, however, it was discussed that the contribution from the latter part may be negligible when the frequencies of these two fields differ by many orders of magnitude, hence preserving the total optical power. We also discussed the extension of this theory for using in analysis of optomechanical cavities. Application examples to non-reciprocal light transmission inside an optomechanical waveguide, and also conceptual design of optomechanical switches were discussed.

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