Electromagnetic field quantization and quantum optical input-output relation for grating

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A quantization scheme is developed for the radiation and higher order electromagnetic fields in one dimensional periodic, dispersive and absorbing dielectric medium. For this structure, the Green function is solved based on the plane wave expansion method, thus the photon operators, commutation relations and quantum Langevin equations are given and studied based on the Green function approach, moreover, the input-output relations are also derived. It is proved that this quantum theory can be reduced back to that of the predecessors’ study on the homogenous dielectric. Based on this method, we find that the transformation of the photon state through the lossy grating is non-unitary and that the notable non-unitary transformation can be obtained by tuning the imaginary part of the permittivity, we also discussed the excellent quantum optical properties for the grating which are similar to the classical optical phenomena. We believe our work is very beneficial for the control and regulation of the quantum light based on gratings.

In recent years, a significant effort has been devoted to the study on the theory and application of metastructure and metasurface, which are artificial periodic structures with their periodicity perpendicular to the incident direction of light. Based on the dimension of the periodicity, they can be classified as one dimensional (1D) grating and two dimensional variation of such structures. A lot of fundamental study on these structures has been conducted, including band structure, scattering, absorption, nonlinear optical effects, and so on. The extraordinary features, like guided resonance, light bound states in the continuum (BICs), and so on, enable these structure to be applied to many optical processes, for example, hollow-core waveguide, high-Q resonators, surface-normal coupler, vertical-cavity surface-emitting lasers, high-NA planar lenses, surface-normal second-harmonic emission, and so on.

The previous study of metastructure and metasurface focuses on the classical optical properties and presents various and meaningful application in classical optics, but an important question is noticeable, how these structures regulate the quantum electromagnetic (EM) field? To solve this problem we should accomplish the the first two basic tasks which are the EM field quantization in those periodic artificial structures and getting the corresponding input-output relation. There has been extensive research on EM quantization. In ref. 27, a fully canonical quantization scheme which is based on the Hopfield model of a dielectric for the macroscopic EM field in a linear harmonic oscillator bulk material is developed, the EM field is coupled to a harmonic-oscillator polarization field that interacts with a continuum of harmonic oscillator reservoir fields. Another method—the Green function approach—is introduced to solve the quantization problem for the dielectric including loss, which can be regarded as a natural extension of the familiar method of the mode expansion to arbitrary Kramers-Kronig consistent media. The quantization of the radiation field is based on the classical Green function representation of the vector potential, identifying the external sources therein with the noise sources that are necessarily associated with the loss in the medium. However, so far there has not been specific EM quantization theory for the medium with periodic structure.

In our work, the plane-wave expansion (PWE) method, which is applied previously to deal with the classical optical problems for the periodic structures, and the Green function approach are used to accomplish the EM field quantization for 1D periodic, dispersive, and lossy medium. The EM fields in plane wave expansion is introduced to the quantum Maxwell equation and then the Green function in the corresponding bulk system can be calculated, on the basis of these the photon annihilators will be obtained. Moreover, we can study the input-output relation and get more quantum properties by applying this relation. Here the method we used is developed from the mode expansion of photon operators.

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Solving of quantum Maxwell equations for 1D grating. We consider 1D periodic structure (1D photonic crystal) as shown in Fig. 1. In order to quantize the electromagnetic field in this structure we will resolve the quantum Maxwell equations using PWE method. Here the relative permittivity is periodic along the x direction and uniform along the y and z direction, we consider the transverse electric (TE) modes in which the electric field is polarized in the uniform y direction, all possible nonzero EM fields are denoted by \((\hat{H}_x, \hat{E}_y, \hat{H}_z)\). The unit vectors of the primitive lattice and the corresponding reciprocal lattice can be introduced as \(a = a e_x\) and \(b = b e_y = 2\pi/a e_x\), respectively. The operator EM fields can be written as the superposition of plane waves based on the PWE method

\[
\hat{E}_y(x, y, z, \omega) = \sum_j \hat{E}_{jy}(z, \omega) e^{i k_j x},
\]

(1a)

\[
\hat{H}_x(x, y, z, \omega) = \sum_j \hat{H}_{jx}(z, \omega) e^{i k_j x} (\xi = x, z),
\]

(1b)

Noise current density \(\hat{j}_y(r, \omega)\) and corresponding bosonic vector field \(\hat{j}_y(r, \omega)\) can be expressed in a similar way. The periodic relative permittivity can be also expanded as \(\varepsilon(x, y, z, \omega) = \sum_j \varepsilon_j(\omega) e^{i k_j y}\). Here the wave vector is \(k_j = k_x + G_j, G_j = j b\). The integer \(j\) in all the previous expressions is taken as \(j = 0, -1, 1, \ldots, N, N\). In principle, the indices \(j\) should run from \(-\infty\) to \(+\infty\), but in numerical practice, truncation over a certain order is necessary. The number of the values of \(j\) is \(M = 2N + 1\), \(\hat{E}_{jy}(z, \omega)\) and \(\hat{H}_{jx}(z, \omega)\) are expansion coefficients of the electric and magnetic fields, \(\varepsilon_j(x, \omega)\) and \(\hat{j}_{jy}(z, \omega)\) represent expansion coefficients of the relative permittivity, noise current density and corresponding bosonic vector field. It is implicit in equations (1) that the Bloch theorem is satisfied for the one dimensional periodic medium.

In order to solve the electric field in this equation, we rewrite it as the following matrix form

\[
-\frac{\partial^2}{\partial z^2} \hat{E}_{my}(z, \omega) + \sum_n (k_n k_m \delta_{m,n} - \omega^2 \varepsilon \varepsilon_m) \hat{E}_{my}(z, \omega) = i\omega \mu_j \hat{j}_{my}(z, \omega).
\]

(2)

In order to solve the electric field in this equation, we rewrite it as the following matrix form

\[
\begin{pmatrix}
-\frac{\partial^2}{\partial z^2} + P(\omega)
\end{pmatrix} \hat{E}_j(z, \omega) = i\omega \mu_j \hat{j}_j(z, \omega),
\]

(3)

where \(P(\omega)\) is \(M \times M\) matrix, \(\hat{E}_j(z, \omega)\) and \(\hat{j}_j(z, \omega)\) are both one column matrices, \(\hat{E}_j(z, \omega) = \left(\hat{E}_{jy}(z, \omega), \hat{E}_{jz}(z, \omega), \hat{E}_{jy}(z, \omega), \ldots, \hat{E}_{jy}(z, \omega)\right)^T\) and \(\hat{j}_j(z, \omega) = \left(\hat{j}_{jy}(z, \omega), \hat{j}_{jz}(z, \omega), \hat{j}_{jy}(z, \omega), \ldots, \hat{j}_{jy}(z, \omega)\right)^T\), the superscript \(T\) means the transpose of the matrices. We use the Green function method to solve the electric field \(\hat{E}_j(z, \omega)\) in Eq. (3), the Green function \(G(z, z', \omega)\) is a \(M \times M\) matrix, in order to solve it, the Fourier transforms of \(\hat{E}_j(n, \omega)\) and...
\[ \hat{J}(\kappa, \omega) \text{ of } \hat{E}(z, \omega) \text{ and } \hat{J}(z, \omega) \text{ should be introduced. Then we substitute these Fourier decomposition into Eq. (3) and obtain an equation in Fourier space shown as follows} \]

\[ (\kappa^2 I + P(\omega)) \hat{E}(\kappa, \omega) = i \omega \eta \hat{J}(\kappa, \omega). \]  

(4)

The corresponding Green function \( G(\kappa, \kappa', \omega) \) for this equation satisfies

\[ (\kappa^2 I + P(\omega)) G(\kappa, \kappa', \omega) = i \delta(\kappa - \kappa'), \]  

(5)

here the Green function \( G(\kappa, \kappa', \omega) \) is also a \( M \times M \) matrix which is the Fourier transform of \( G(z, z', \omega) \), \( I \) is the identity matrix, \( \hat{E}(\kappa, \omega) \) and \( \hat{J}(\kappa, \omega) \) are one column matrices. The eigenvalues of the matrix \( P(\omega) \) and the \( M \times M \) matrix \( S(\omega) \), whose \( \sigma \) th column \((S_{\sigma\alpha}(\omega), S_{1\alpha}(\omega), S_{2\alpha}(\omega), \ldots, S_{M\alpha}(\omega), S_{0\alpha}(\omega))^T \) is the eigenvector corresponding to the eigenvalue \( -\kappa_\sigma^2(\omega) \), can be obtained simultaneously, \( \kappa_\sigma(\omega) \) is the wavevector along \( z \) direction. The matrix \( S(\omega) \) satisfies

\[ \sum_{\sigma=0}^{N} S_{\sigma\alpha}(\omega) S_{\sigma\beta}(\omega) \delta(\kappa - \kappa') = \delta_{\alpha\beta}\delta(\kappa - \kappa'). \]  

(6)

Then the Green function \( G(\kappa, \kappa', \omega) \) in Eq. (5) can be calculated based on Eq. (6)

\[ G_{\alpha\beta}(\kappa, \kappa', \omega) = \sum_{\sigma=0}^{N} \frac{S_{\sigma\alpha}(\omega) S_{\sigma\beta}(\omega) \delta(\kappa - \kappa')}{(\kappa - \kappa_\sigma - i\delta)(\kappa + \kappa_\sigma + i\delta)} \]  

(7)

where \( \delta \) is a positive infinitesimal, the dependence on \( \omega \) is implicit for \( \kappa_\sigma(\omega) \) and \( S(\omega) \). The Green function \( G(z, z', \omega) \) can be calculated by integrating \( G(\kappa, \kappa', \omega) \) over \( \kappa \) and \( \kappa' \)

\[ G_{\alpha\beta}(z, z', \omega) = i \sum_{\sigma=0}^{N} \frac{S_{\sigma\alpha}(\omega) S_{\sigma\beta}(\omega) e^{i\kappa_\sigma(z - z')}}{2\kappa_\sigma}. \]  

(8)

the residue theorem is used in the calculation of this integral. Based on this Green function the field \( \hat{E}_{\alpha\beta}(z, \omega) \) can be solved

\[ \hat{E}_{\alpha\beta}(z, \omega) = i \mu_\omega \sum_{\sigma} S_{\sigma\alpha}(\omega) \hat{e}^{i\beta_\sigma z_\sigma} (e^{i\beta_\sigma z_\sigma} + e^{-i\beta_\sigma z_\sigma}) \hat{J}_\sigma(z, \omega), \]  

(9)

here the amplitude operators \( \hat{\sigma}_\sigma^+(z, \omega) \) and \( \hat{\sigma}_\sigma^-(z, \omega) \) are introduced, which propagate forward (along \( +z \) direction) and backward (along \( -z \) direction), respectively,

\[ \hat{\sigma}_\sigma^+(z, \omega) = i \int_0^z d\tau \sum_{\kappa} \frac{i S_{\sigma\alpha}(\omega) e^{-i\kappa_\sigma \tau\kappa_\sigma}}{2\kappa_\sigma} e^{i\kappa_\sigma(z - \tau) \hat{J}_\sigma(z', \omega)}, \]  

(10a)

\[ \hat{\sigma}_\sigma^-(z, \omega) = i \int_0^\infty d\tau \sum_{\kappa} \frac{i S_{\sigma\alpha}(\omega) e^{-i\kappa_\sigma \tau\kappa_\sigma}}{2\kappa_\sigma} e^{i\kappa_\sigma(z - \tau) \hat{J}_\sigma(z', \omega)}, \]  

(10b)

where we assume the wave vector \( \kappa_\sigma = \beta_\sigma + i\gamma_\sigma \), \( \beta_\sigma \) and \( \gamma_\sigma \) are the real and imaginary parts of \( \kappa_\sigma \).  

**Annihilation and creation operators.** Based on the explicit expressions of amplitude operators, we have also studied the spatial evolution of the amplitude operators which is governed by quantum Langevin equations (see Supplementary Material), where the quantum noise associated with the damping is taken into account by operator Langevin noise sources. After consideration of the commutation relations of the operator noise current densities, we can get the commutation relations of the amplitude operators (see Supplementary Material), from the results we can see that the commutation relations of the amplitude operators with different orders may not be zero. A special case is considered \( z = z' \) and then we define a matrix \( U_{\alpha\beta}(\omega) \) in this case

\[ [\hat{\sigma}_\alpha^+(z, \omega), \hat{\sigma}_\beta^+(z', \omega')] = U_{\alpha\beta}(\omega) e^{\pm i\beta_\sigma \gamma_\sigma} \delta(\omega - \omega'). \]  

(11)

The commutation relations of the photon annihilation operators with different orders should be equal to zero, so we introduce the photon annihilation operators \( \hat{\sigma}_\alpha^+(z, \omega) \) and \( \hat{\sigma}_\beta^+(z, \omega) \), which are the linear superposition of the amplitude operators \( \hat{\sigma}_\alpha^+(z, \omega) \) and \( \hat{\sigma}_\beta^+(z, \omega) \), respectively,

\[ \hat{\sigma}_\alpha^+(z, \omega) e^{\pm i\beta_\sigma \gamma_\sigma} = \sum_{\kappa} [X^+(\omega)]_{\kappa\sigma} \hat{\sigma}_\kappa^+(z, \omega) e^{\pm i\beta_\kappa \gamma_\kappa}. \]  

(12)

The matrixes of superposition coefficients \( X^+(\omega) \) and \( X^- (\omega) \) are determined by the commutation relations of the bosonic photon annihilation and creation operators

\[ [\hat{\sigma}_\alpha^+(z, \omega), \hat{\sigma}_\beta^+(z, \omega')] = \delta_{\alpha\beta} e^{-i(\beta_\alpha \omega_\alpha - \beta_\beta \omega_\beta)} \delta(\omega - \omega'). \]  

(13)

Substituting in the left of the commutation relations in Eq. (13) for the photon operators the superposition forms (12), the coefficients \( X^+(\omega) \) and \( X^- (\omega) \) can be determined by \( U(\omega) \).
It is clearly seen from Eq. (14) that $X^+ (\omega)$ is equal to $X^- (\omega)$ ($X^+ (\omega) = X^- (\omega) = X(\omega)$). So far, the EM field quantization in one-dimensional photonic crystal is fully completed, the final form of the electric field can be written as in matrix

$$[X^\pm (\omega)]^{-1} U(\omega) [X^\pm (\omega)]^{-1T} = I. \quad (14)$$

It is clearly seen from Eq. (14) that $X^+ (\omega)$ is equal to $X^- (\omega)$ ($X^+ (\omega) = X^- (\omega) = X(\omega)$).

Quantum optical input-output relation for grating. Now we turn to the problem of propagation of the quantized field through 1D periodic dielectric slab—1D grating—embedded in two semi-infinite homogeneous dielectrics, which is shown in Fig. 2. The dielectric function is expressed as

$$\varepsilon(x, \omega) = \Theta(-z - l/2)\varepsilon^1(\omega) + [\Theta(z + l/2) - \Theta(z - l/2)]\varepsilon^2(x, \omega) + \Theta(z - l/2)\varepsilon^3(\omega). \quad (16)$$

the superscripts 1, 2, 3 represent three corresponding regions.

The input-output relation of annihilation operators in transfer matrix form for the grating can be obtained by using EM boundary condition and solution of quantum Langevin equation (see Supplementary Material)

$$\begin{bmatrix} \hat{a}^+ (l/2, \omega) \\ \hat{a}^- (l/2, \omega) \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{bmatrix} \begin{bmatrix} \hat{a}^+ (-l/2, \omega) \\ \hat{a}^- (-l/2, \omega) \end{bmatrix} + \begin{bmatrix} t_{11} & t_{12} \\ t_{21} & t_{22} \end{bmatrix} \begin{bmatrix} \hat{G}^+_n (\omega) \\ \hat{G}^-_n (\omega) \end{bmatrix}, \quad (17)$$

here the columns $\hat{G}^+_n (\omega)$ and $\hat{G}^-_n (\omega)$ are associated with the grating. The commutation relations of $\hat{G}^+_n (\omega)$ with different orders may not be zero, in light of mentioned theoretical discussion we construct the new operators $\hat{G}^+_n (\omega)$ and $\hat{G}^-_n (\omega)$ associated with the slab which satisfy the bosonic commutation relations. Firstly, we define $\hat{G}^0_n (\omega)$ and $\hat{G}^0_n (\omega)$ to ensure that they commute with each other

$$\hat{G}^0_n (\omega) = -\hat{G}^-_n (\omega) \pm \hat{G}^+_n (\omega). \quad (18)$$

After some calculation, the related commutation relations are listed in the following, moreover, the matrix $V$ is introduced further.
Secondly, we construct new operators $\hat{g}_n^{0+}(\omega)$ and $\hat{g}_n^{0-}(\omega)$ as linear superposition of operators $\hat{G}_n^{0+}(\omega)$ and $\hat{G}_n^{0-}(\omega)$ in the similar way to construct the photon operators

$$\hat{g}_n^{0\pm}(\omega) = \sum_{n} Y_n^{0\pm}(\omega) k_n^{0\pm}(\omega),$$

(20)

The new operators should fulfill the bosonic commutation relations

$$[\hat{g}_m^{\pm}(\omega), \hat{g}_n^{=}(\omega')] = \delta_{mn}\delta(\omega - \omega').$$

(21)

Similarly, the coefficients of $Y^+(\omega)$ and $Y^-(\omega)$ can be determined from the above equations by substituting the Eqs. (20) into (21)

$$[Y^+(\omega)]^{-1} V^+(\omega) [Y^+(\omega)]^{-1\dagger} = 1.$$

(22)

Finally, the quantum optical input-output relation expressed in the transfer matrix form can be transformed to the scattering matrix $Q_{mn}(mn = 11, 12, 21, 22)$.
So far we construct the relation between the output annihilation operators $\hat{a}^\dagger_{l,\omega}$ and the input annihilation operators $\hat{a}^\dagger_{l,\omega}$ and the bosonic excitations associated with the slab $\hat{g}^\dagger_{\omega}$, $\hat{g}^\dagger_{\omega}$. The new operators $\hat{g}^\dagger_{\omega}$ and $\hat{g}^\dagger_{\omega}$ play the role of the noise sources associated with the damping in the input-output relation. When we consider the special case of homogeneous dielectric, the input-output relation and related commutation relations can be also derived back to the previous study\textsuperscript{37,38}.

Then we can derive the commutation relations between the output photon operators based on the input-output relation together with the known commutation relations between the input photon operators. After deliberate and straightforward calculation the results can be written in matrix form

$$
\begin{pmatrix}
\hat{a}^\dagger_{\frac{1}{2},\omega} \\
\hat{a}^\dagger_{-\frac{1}{2},\omega}
\end{pmatrix} =
\begin{pmatrix}
Q_{11} & Q_{12} \\
Q_{21} & Q_{22}
\end{pmatrix}
\begin{pmatrix}
\hat{a}^\dagger_{\frac{1}{2},\omega} \\
\hat{a}^\dagger_{-\frac{1}{2},\omega}
\end{pmatrix}
+ \begin{pmatrix}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{pmatrix}
\begin{pmatrix}
\hat{g}^\dagger_{\omega} \\
\hat{g}^\dagger_{\omega}
\end{pmatrix}
$$

(23)
Here the matrixes shown in the above equation are defined as 
\[
\left( \begin{array}{cc}
c_{11} & c_{12} \\
c_{21} & c_{22}
\end{array} \right) = \left( \begin{array}{cc}
Q_{11} & Q_{12} \\
Q_{21} & Q_{22}
\end{array} \right) + \left( \begin{array}{cc}
A_{11} & A_{12} \\
A_{21} & A_{22}
\end{array} \right),
\]
(24)

Figure 5. The absorption, \(c_{11,00}\) and \(c_{12,00}\) for the grating when the geometric parameters are changed: (a–c) show the absorption, \(c_{11,00}\) and \(c_{12,00}\) as functions of the reduced wavelength \(\lambda/\Lambda\) and the reduced thickness \(l/\Lambda\), the width of the grating is chosen as \(w = 0.6\Lambda\). (d–f) depict the absorption, \(c_{11,00}\) and \(c_{12,00}\) as functions of the reduced wavelength \(\lambda/\Lambda\) and the filling factor \(w/\Lambda\), the thickness of the grating is chosen as \(l = 1.75\Lambda\). For all these cases, the relative permittivity of the grating is \(\varepsilon = (4, 0.1)\) and the incident photons propagate normally \(\theta = 0^\circ\).
seen from Figs. 3(b), 4(b,c), that means the output photons satisfy bosonic commutation relation and the annihilation operators for different channels commute with each other, these results coincide with the former work. For gratings, only when it is lossless, $c_{11,00} = 1$ and $c_{12,00} = 0$, which can be seen from Fig. 3(d), when it is lossy, these equations are not true in this case, that is to say, $c_{11,00} ≠ 1$ and $c_{12,00} ≠ 0$, which can be seen from 4(e,f). After comparing the four different models, we find that the physical origin of this inequality is that the excitations, $\hat{g}_{m}^h(\omega)$ and $\hat{g}_{m}^v(\omega)$, in different orders interact with each other. Not only that, from Fig. 4(d–f) we also find that near the guided resonance, which is the Fano resonance in our optical model, obvious resonance and deviation of $c_{11,00}$ and $c_{12,00}$, the deviation means that the departure of $c_{11,00}$ value from 1 and $c_{12,00}$ value from 0. It can be also clearly seen that at the reduced wavelength $\lambda / \Lambda > 1.5$, there is no guided resonance, while there is also no resonance for $c_{11,00}$ and $c_{12,00}$ and the deviation decreases.

The Heisenberg picture is implied in the quantization theory, when the theory is converted to Schrödinger picture, we can understand the phenomenon further, which is the deviation of the bosonic commutation relations for the output photon operators in the lossy grating. In the Schrödinger picture, the evolution operator is no longer unitary with respect to the radiated order which can be derived from the input–output relation40,41, so the transformation of the quantum states is non-unitary. From Fig. 4(e,f) we can see that the phenomenon of deviation is very small ($\sim 10^{-3}$).

Now we tune $c_{11,00}$ and $c_{12,00}$, which describe the transformation of the photon states, by change the parameters in our model. Compared to the classical optics the Fano resonance can appear in the grating for quantum light which can be seen from Fig. 5(a,d), near the resonant absorption is notable. The peak and valley of the absorption are developed because of their excellent optical properties42,43, we believe that the grating can be applied in various areas of quantum optics, such as propagation of non-classical light, quantum state transformation, spontaneous emission of a nearby scatter and so on, these will be our next tasks.

Conclusion

We give the Green function and the EM field quantization for 1D periodic, dispersive and absorbing dielectric bulk medium firstly. The EM field are expanded in plane waves and are inserted to the quantum Maxwell equations, the Green function is solved, furthermore the electric field is quantized and the amplitude annihilators are established. The commutation relations of these amplitude operators in our periodic bulk system are calculated out based on the previous known commutation relations of the operator noise current density, we find that the amplitude operator don’t commute with the its Hermite operator with different order, which is quite different
from the homogeneous dielectric case. Then we construct the photon annihilation operators by linear superposition of the amplitude operators. The quantum Langevin equations which determine the spatial evolution of the amplitude operators in our bulk system are provided and studied.

The quantum input-output relation for the grating is also derived, the output field operators can be described in terms of input field operators and noise sources associated with the loss in the gratings. We find that the conventional commutation relations are satisfied, $c_{1,0}^{\dagger} = [\hat{a}_{0}^{\dagger}, (U/2, \omega), \hat{a}_{0}^{\dagger} + (U/2, \omega)] = 1$ and $c_{1,0} = [\hat{a}_{0}^{\dagger}, (U/2, \omega), \hat{a}_{0}^{\dagger} - (U/2, \omega)] = 0$ for uniform slab or lossless grating, but for lossy grating, these relations do not hold, these phenomena originate from the interaction between the output photon in radiation order and the excitations in higher orders. The excellent quantum optical properties of the grating are also found and discussed. We believe our work is very beneficial for the control and regulation of the quantum light based on gratings.

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Author contributions
Tiecheng Wang conceived the idea, performed the research and wrote the manuscript.

Competing interests
The author declares no competing interests.

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