

**GREEN'S FUNCTION METHODS IN
PHOTONIC CRYSTALS AND CLUSTERS**

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Abstract: In the semiclassical framework, resonant photonic crystals and clusters computation requests to solve self-consistently the Schroedinger-Maxwell coupled equations in order to study linear and non-linear optical properties of mesoscopic materials. In a non-local spatially periodic medium the electromagnetic propagation properties will be computed by transforming integral-differential Maxwell equations in integral equations, therefore, the Green's function formalism usually take a crucial role in the optical computation.

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1. Introduction

Diffraction phenomena are at basis of many interesting optical properties shown by the light propagation in complex systems; moreover, they take a crucial role in the tailoring of optical devices, allowing the control of the local photon density of states.

Light propagation in periodic systems, studied at very beginning of modern optics to explain anomalous light propagation often observed in grating [10], [9]

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has received nowadays a very large effort in the “photonic crystals” framework as suggested by S. John [3] and E. Yablonovich [11].

Optical properties of photonic crystals are usually described as diffractive phenomena in the zone of the electronic gap of the material systems where dissipative effects can be neglected. In this case, macroscopic Maxwell equations and real dielectric functions are usually used for the calculation of the photonic dispersion curves.

Since localized electronic transitions (deep and shallow impurities) or extended states (Frenkel and Wannier excitons) usually appear in the electronic gap in resonance with photonic states the so called “resonant photonic crystals” can be considered, and dissipative effects cannot be any more neglected. In this case, microscopic framework and non-local susceptibility must be used, and optical properties are usually computed in the semiclassical framework by solving self-consistently Schroedinger and Maxwell equations in the effective mass approximation [5], [2].

The aim of the present work is to discuss the main frameworks and formula, based on the Green's function formalism, adopted for computing the optical properties of spatially periodic mesoscopic superstructures.

In Section 2 the microscopic basis of the macroscopic Maxwell's equations is briefly summarized. In Section 3 we derive the Green's function for computing exciton-photon interaction (polaritons), in semiclassical framework, for spatially periodic systems, with linear non local susceptibility (resonant photonic crystals). Conclusions are given in Section 4.

2. Maxwell's Equations and the Related Dyadic Green's Functions

In their microscopic form, the Maxwell's equations are described by the electric (\mathbf{E}) and magnetic induction (\mathbf{B}) fields:

$$\nabla \times \mathbf{B} - \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} = \frac{4\pi}{c} \mathbf{j}, \quad \nabla \cdot \mathbf{E} = 4\pi\rho, \quad \nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0, \quad \nabla \cdot \mathbf{B} = 0, \quad (1)$$

where ρ and \mathbf{j} are the charge and current densities related by the continuity relationship: $\dot{\rho} = -\nabla \cdot \mathbf{j}$. In order to obtain the macroscopic Maxwell's equations from the microscopic ones, it is necessary to perform macroscopic averaging of microscopic variables over a volume larger than atomic scale but smaller than light wavelength. In this case the charge and current densities can be written as summation of their true (ρ_o, \mathbf{j}_o) and induced (ρ_p, \mathbf{j}_p) components:

$\rho_p = \nabla \cdot \mathbf{P} + \nabla \nabla : \mathbf{Q}$ and $\mathbf{j}_p = c \nabla \times \mathbf{M} + \dot{\mathbf{P}} - \nabla \cdot \dot{\mathbf{Q}}$; where \mathbf{P} and \mathbf{M} are the polarization and magnetization dipole densities and \mathbf{Q} is the second rank quadrupole tensor.

By substitution in equations (1) we can obtain the macroscopic Maxwell's equations:

$$\nabla \cdot (\mathbf{E} + \mathbf{P} - \nabla \cdot \mathbf{Q}) = \nabla \cdot \mathbf{D} = 4\pi \rho_o, \quad (2a)$$

$$\nabla \times (\mathbf{B} - c\mathbf{M})/c - (\dot{\mathbf{E}} + \dot{\mathbf{P}} - \nabla \cdot \dot{\mathbf{Q}})/c = \nabla \times \mathbf{H}/c - \dot{\mathbf{D}}/c = 4\pi \mathbf{j}_o/c. \quad (2b)$$

Now, let us consider the Maxwell's equation for the electric field:

$$\nabla \times [\nabla \times \mathbf{E}(r, t)] + \ddot{\mathbf{E}}/c^2 = -4\pi \dot{\mathbf{j}}(r, t)/c^2, \quad (3a)$$

where the ω -Fourier component is:

$$\nabla \times [\nabla \times \mathbf{E}(r, \omega)] - \omega^2 \mathbf{E}/c^2 = -i 4\pi \omega \mathbf{j}(r, \omega)/c^2. \quad (3b)$$

The dyadic Green's function, that relates the electric field and the current density, must satisfy the following equation:

$$\nabla \times [\nabla \times G(r, r'; \omega)] - \omega^2 G(r, r'; \omega)/c^2 = 4\pi I \delta(r - r'). \quad (4)$$

In order to clarify the connection between transverse field and current density, the electric and the magnetic induction fields are expressed in terms of the scalar electric potential (φ) and of the magnetic potential vector (\mathbf{A}) by adopting the gauge of Coulomb ($\nabla \cdot \mathbf{A} = 0$): $\mathbf{E} = -\dot{\mathbf{A}}/c - \nabla \varphi$ and $\mathbf{B} = \nabla \times \mathbf{A}$.

The scalar potential φ is:

$$\varphi(r, t) = \int_{-\infty}^{\infty} dr' \frac{\rho(r', t)}{|r - r'|} \quad (5a)$$

and its ω -Fourier component, by using the continuity relationship, is:

$$\varphi(r, \omega) = -\frac{i}{\omega} \int_{-\infty}^{\infty} dr' \frac{\nabla' \cdot \mathbf{j}(r', \omega)}{|r - r'|}, \quad (5b)$$

that substituted in equation (3b) gives:

$$-(\omega^2/c^2 + \nabla^2) A - \frac{1}{c} \nabla \int dr' \frac{\nabla' \cdot \mathbf{j}(r', \omega)}{|r - r'|} = \frac{4\pi}{c} \mathbf{j}(r, \omega). \quad (6)$$

That can be also written as [2]:

$$-(\omega^2/c^2 + \nabla^2) A(r, \omega) = \frac{4\pi}{c} j(r, \omega) + \frac{1}{c} \int_{-\infty}^{\infty} dr' \frac{\nabla' \nabla' \cdot \mathbf{j}(r', \omega)}{|r - r'|}. \quad (7)$$

The scalar Green's function related to the $(\omega^2/c^2 + \nabla^2)$ operator is:

$$g(r, r') = \exp [i|r - r'| \omega/c] / |r - r'|. \quad (8)$$

The solution of equation (2) is obtained in the integral form:

$$\begin{aligned} A(r) &= A^o(r) + \frac{1}{c} \int_{-\infty}^{\infty} dr' g(r, r') j(r') + \frac{1}{4\pi c} \int_{-\infty}^{\infty} dr' \int_{-\infty}^{\infty} dr'' g(r', r'') \frac{\nabla'' \nabla'' \cdot \mathbf{j}(r'')}{|r' - r''|} \\ &= A^o(r) + \frac{1}{c} \int_{-\infty}^{\infty} dr' G_p(r, r') \mathbf{j}(r'), \end{aligned} \quad (9)$$

that allows us to define the tensorial photon Green's function $G_p(r, r')$.

3. Green's Function Method for Photonic Crystals and Clusters Computation

3.1. Polariton Green's Function for 1D Multilayer System

Let us consider a 1D heterostructure constituted of N dielectric layers oriented as the z -axis of a Cartesian system, and in presence of electronic transitions (confined Wannier exciton) in resonance with light energy.

The real background dielectric function is:

$$\varepsilon_B(z) = \varepsilon_o \theta(-z) + \sum_{\ell=1}^N \varepsilon_{\ell} \theta(z - L_{\ell-1}) \theta(L_{\ell} - z) + \varepsilon_{N+1} \theta(z - L_N). \quad (10)$$

L_{ℓ} and ε_{ℓ} are the layer thickness and the dielectric function of the ℓ -layer respectively, and $\theta(z)$ is the Heaviside step function.

The polarization vector \mathbf{P} can be given in term of the background dielectric B and linear L exciton polarizations [5] as: $\mathbf{P} = \mathbf{P}^B + \mathbf{P}^L$, where:

$$\mathbf{P}^{(B)} = \varepsilon_B(z) \mathbf{E} / 4\pi, \quad (11)$$

$$\mathbf{P}^{(L)} = \sum_n \frac{S_o(\omega)}{E_n - \hbar\omega - i\Gamma} \Psi_n^*(z) \int_L \Psi_n(z') \mathbf{E}(z') dz'. \quad (12)$$

Ψ_n and E_n are the eigenfunction and the selfenergy of the quantum confined exciton n -state, while $S_o(\omega)$ and Γ are the valence-conduction dipole transition and non-radiative broadening respectively.

By taking: $\varepsilon_B(k_{//}, z) = \varepsilon_B(z) - k_{//}^2/q^2$, where $k_{//}$ is the in-plane wave vector and $q^2 = \omega^2/c^2$, the Maxwell's equation is:

$$\frac{d^2 E(z; k_{//})}{dz^2} + q^2 \varepsilon_B(k_{//}, z) \mathbf{E}(z; k_{//}) = -4\pi \frac{\omega^2}{c^2} \mathbf{P}^{(L)}(z; k_{//}). \quad (13)$$

For an exciton located in ℓ' -layer, the differential equation of the Green's

function is:

$$D_z G_p(k_{//}; z, z') + 4\pi \sum_n S_n(\omega) \Psi_n^*(z) \int_{L_{\ell'}} G_p(k_{//}; z', z'') \Psi_n(z'') dz'' = -4\pi q^2 \delta(z - z'), \quad (14)$$

where $L_{\ell'}$ is the range of integration inside the ℓ' -layer, $k_{\ell'} = [q^2 \varepsilon_{\ell'} - k_{//}^2]^{1/2}$ is the z-component of wave vector in the same layer and D_z is the differential operator of Maxwell's equation: $D_z = \left[\frac{d^2}{dz^2} + q^2 \varepsilon_B(k_{//}, z) \right]$.

Notice that, in a planar periodic multilayer photon field, exciton and their mixed state (polariton) show the same value of the in-plane $k_{//}$ wave vector.

Now, by taking into account the following identities:

$$D_z^{-1} \delta(z - z') = -\frac{1}{4\pi} g_{\ell'}(k_{//}; z, z'), \quad (15)$$

$$D_z^{-1} \Psi_n^*(z) = -\frac{1}{4\pi} \int_{L_{\ell'}} g_{\ell'}(k_{//}; z, z') \Psi_n^*(z') dz', \quad (16)$$

$$\Psi_n^*(z) = -\frac{1}{4\pi} \int_{L_{\ell'}} D_z [g_{\ell'}(k_{//}; z, z')] \Psi_n^*(z') dz', \quad (17)$$

and by applying the D_z^{-1} to the former differential equation, the polariton Green's function is:

$$G_p(k_{//}; z, z') - \sum_n S_n(\omega) \int_{L_{\ell'}} g(k_{//}; z, z''') \Psi_n^*(z''') dz''' \times \int_{L_{\ell'}} G_p(k_{//}; z', z'') \Psi_n(z'') dz'' = g(k_{//}; z, z'). \quad (18)$$

The kernel of the integral equation is degenerate, and this allows us to transform the integral equation (18) in an algebraic linear system by applying the integral operator

$$\int_{L_{\ell'}} dz \Psi_m(z) \cdot \int_{L_{\ell'}} G_p(k_{//}; z, z') \Psi_m(z) dz - \sum_n S_n(\omega) \int_{L_{\ell'}} dz \Psi_m(z) \int_{L_{\ell'}} dz''' g(k_{//}; z, z''') \Psi_n^*(z''') \times \int_{L_{\ell'}} G_p(k_{//}; z', z'') \Psi_n(z'') dz'' = \int_{L_{\ell'}} g(k_{//}; z, z') \Psi_m(z) dz. \quad (19)$$

Finally, by substituting in the former equation the following ones:

$$\int_{L_{\ell'}} G_p(k_{//}; z, z') \Psi_m(z) dz = H_m(k_{//}, z'), \quad (19)$$

$$\int_{L_{\ell'}} g(k_{//}; z, z') \Psi_m(z) dz = h_m(k_{//}, z'), \quad (20)$$

$$S_n(\omega) \int_{L_{\ell'}} dz \Psi_m(z) \int_{L_{\ell'}} g(k_{//}; z, z''') \Psi_n^*(z''') dz''' = D_{mn}(k_{//}, \omega), \quad (21)$$

we obtain a linear algebraic system:

$$\sum_n [\delta_{mn} - D_{mn}(k_{//}, \omega)] H_n(k_{//}, z') = h_m(k_{//}, z'), \quad (22)$$

whose solutions allow us to write down the polariton Green's function $G_p(k_{//}; z, z')$ as a function of photon Green's function $g(k_{//}; z, z')$:

$$G_p(k_{//}; z, z') = g(k_{//}; z, z') + \sum_n S_n(\omega) H_n(k_{//}, z') \int_{L_{\ell'}} dz'' g(k_{//}; z, z'') \Psi_n^*(z''). \quad (23)$$

The photon Green's function $g(k_{//}; z, z')$ must satisfy the following equation:

$$\frac{d^2 g(k_{//}; z, z')}{dz^2} + k_z^2 g(k_{//}; z, z') = -4\pi \frac{\omega^2}{c^2} \delta(z - z'). \quad (24)$$

The solution for the general ℓ -layer is:

$$g_\ell(k_\ell, z, z') = a_\ell \exp(ik_\ell z) + b_\ell \exp(-ik_\ell z) \quad (26a)$$

while for the ℓ' -layer, where the exciton is, we must add a further term:

$$g_{\ell'}(k_{//}, z, z') = a_{\ell'} \exp(ik_{\ell'} z) + b_{\ell'} \exp(-ik_{\ell'} z) + \frac{2\pi}{ik_{\ell'}} q^2 \exp(ik_{\ell'} |z - z'|). \quad (26b)$$

The coefficients $\{a_\ell, b_\ell\}$ are obtained by the condition that both the function $g(k_{//}, z, z')$ and its first derivative are continuous across each interface of the multilayer, see [1], [8]. Moreover, since the field is produced from the z' source point, no incoming field is produced outside. Therefore, we can set $a_0 = 0$ and $b_{N+1} = 0$, so that the number of unknown coefficients $\{a_\ell, b_\ell\}$ reduce to $2N + 2$. It is equal to the number of boundary conditions and this allows us to uniquely determine the set $\{a_\ell, b_\ell\}$ so to obtain both the photonic and the polaritonic Green's function of the multilayer for a $k_{//}$ -channel.

3.2. Green Function for a 1D Laterally Patterned Optical Multilayer

The EM field in a multilayer, where 1D (or 2D) periodicity is present at the $\ell = s$ layer [5], can be computed by using the former polaritonic Green's solution of the equation (23) for each $k_{//} = q_{//} + G$ channel, where $G = n 2\pi/d$; $n = 0, \pm 1, \pm 2, \dots, \pm N$, and d is the lateral spatial periodicity ($q_{//}$ is chosen in the first 1D Brillouin's zone).

Specializing the formula for 1D lateral polarization \mathbf{P}_{lat} along x-axis $q_{//} = q_x$:

$$\mathbf{P}_{lat}(z, q_{//} + G) = \sum_{G'} \chi_g(G - G') E(q_{//} + G', z). \tag{27}$$

$\chi(G - G')$ is the Fourier component of the susceptibility:

$$\chi_g(G - G') = \frac{2}{d} \Delta\varepsilon \frac{\sin [(G - G') L_x/2]}{G - G'}, \tag{28}$$

where $\Delta\varepsilon = \varepsilon_2 - \varepsilon_1$ is the binary dielectric contrast and L_x the lateral wire thickness of the grating. The integral-differential Maxwell equation is:

$$D_z E(z; q_{//} + G) + 4\pi q^2 \left[\mathbf{P}^{(L)}(z; q_{//} + G) + \sum_{G'} \chi_g(G - G') E(z, q_{//} + G') \right] = 0, \tag{29}$$

where the reciprocal lattice vectors $\{G\}$ are mixed by the lateral periodicity.

The electromagnetic field can be computed by solving the equivalent Lippmann-Schwinger integral equation:

$$E(z, q_{//} + G) = E^o(z, q_{//} + G) + \sum_{G'} \int_{\ell=s} G_p(z, z'; q_{//} + G) \chi_g(G - G') E(z', q_{//} + G') dz', \tag{30}$$

where the polariton multilayer Green's function of equation (23) is used. The explicit solution given in algebraic analytic form is reported in [8].

3.3. Polariton Green's Function for 3D Resonant Photonic Crystal and Cluster

Now, we would like to underline that the analytic solution of equation (29) describes the optical properties of a complex 1D multilayer (along z-axis) with 1D and/or 2D lateral periodicity (along x or x,y directions). Moreover, since

the former solution is essentially one-dimensional in character (along z-axis), two different generalization are at hand, namely:

i) We can consider the former system as the “building block” of a mesoscopic uniaxial resonant photonic crystals. The optical properties are obtained by using the translation symmetry operator (along z-axis) as for the generalized Kroening-Penney model. This method is usually adopted in the layer-by-layer calculation in surface science.

ii) We can compute the tensor Green's function of the former planar cluster of N-layers by using the independent right and left solutions along z-axis of the electric field (see equation (29)) and applying the standard method given in [4].

4. Conclusions

The main concepts in the optical properties of mesoscopic systems are briefly highlighted and Green's function formula, well suited for computing optical properties in spatially periodic systems, are explicitly summarized.

The Green's function method illustrated before allows us to obtain analytical solutions for the linear and non-linear optical response of spatially periodic system when extended or localized resonant states are present (resonant photonic crystals).

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