Semiclassical theory of excitonic polaritons in a planar semiconductor microcavity

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(March 24, 2022)

Abstract

We present a comprehensive theoretical description of quantum well exciton-polaritons imbedded in a planar semiconductor microcavity. The exact non-local dielectric response of the quantum well exciton is treated in detail. The 4-spinor structure of the hole subband in the quantum well is considered, including the pronounced band mixing effect. The scheme is self-contained and can be used to treat different semiclassical aspects of the microcavity properties. As an example, we analyze the "selection" rules for the exciton-cavity mode coupling for different excitons.
I. INTRODUCTION

Since the first experiment on quantum well (QW) excitonic polaritons in the semiconductor microcavity (SMC), extensive experimental and theoretical studies have been conducted on excitonic polaritons in QW’s and multiple QW’s embedded in an SMC, and even bulk excitonic polaritons in an SMC. The SMC exciton-polariton was first described by so-called linear dielectric model which was originally proposed for atoms in a microcavity. Since then, most analysis on the microcavity problem has been more or less based upon the assumed analogy between excitons and atoms. The non-locality of the dielectric response of the exciton in a QW and the intricacy of real excitons due to the complex structure of the valence band has not been treated seriously.

In fact, excitons differ from an atomic excitation in that they are a sort of excitation from electrons in the valence band confined by the QW’s barriers. The excitonic polariton is essentially a quantum many-body effect and can be understood to be a result of the medium’s polarization. In the calculation of the dielectric response to light propagation in a QW, we have translational invariance only in the plane perpendicular to the growth direction, so the nonlocality of the dielectric response along the growth direction should be carefully treated. This makes the problem of a QW exciton embedded in an SMC non-trivial. In particular, the barrier confinement effect in association with the 4-component spinor-like hole wave function should appear in the nonlocal dielectric response. The confinement induces hybridization between heavy and light hole subbands, which sometimes plays a nontrivial role at the top region (Γ-point) of the valence band and has interesting observable consequences for the optical transitions of the excitons in a QW. This makes the nonlocal dielectric response of the QW more complex. To our knowledge, the non-locality of QW exciton-polariton has been considered for the simplified exciton model, while the real QW exciton model including non-locality and subband mixing effects has not yet been considered seriously, especially in a microcavity environment. On the other hand, although the effect of such hybridization induced exciton is not very strong, the exciton-photon coupling is
greatly enhanced in the microcavity. Thus it is interesting to investigate the nature of such hybridization induced QW excitonic polaritons in the SMC environment.

Based upon the above considerations, in this paper we provide a self-consistent semiclassical description of the excitonic polaritons in a QW embedded in an SMC, in which the hole subband hybridization, the nonlocality induced by the QW barrier confinement and the boundary conditions for the SMC in connection with distributed Bragg reflectors (DBR’s) are all consistently taken into account. The light field is treated semiclassically but the polarization of the medium in the QW is treated in the context of quantum many-body theory with the electromagnetic wave-electron-hole interaction, so that the description of the effective coupling between light and excitons does not need any phenomenological input “coupling constant”. The only input parameters are the width of the exciton levels. The calculated Rabi splitting of conventional excitonic polaritons could be considered as an improvement to the so-called dielectric model in which the photon-exciton coupling constant is estimated using the electric field of a cavity mode and and the oscillator strength of an exciton. We will show also the complexity in introducing such an effective oscillator strength due to the coupling of the motion along or perpendicular to the growth directions for the hybridization induced polaritons. As an interesting effect of the barrier confinement induced electron and hole envelope wave functions for a system with a pair of symmetric DBR’s, we apply parity symmetry analysis along the growth direction to the DBR’s and the SMC confined QW, and obtain a kind of selection rule for excitonic polaritons in the well, which is also quite useful for finding the hole subband hybridization induced polaritons. As an application of our scheme, we have calculated the reflection spectrum for several different excitons and for different incident angles, and have obtained some interesting results, which will be published elsewhere. Here we only discuss the formal aspects of our approach.

Since this topic is in an interdisciplinary field between condensed matter physics and quantum optics, we present our discussion in a self-contained way for readers in both fields. This paper is organized as follows. In Sec. II., we formulate the description of the excitonic polaritons in a QW embedded in an SMC in terms of a propagating electromagnetic
field, while the SMC is further confined by a pair of DBR’s. The basic spirit of its classical
electrodynamic aspect mainly follows ref.26, but the crucial difference is in the physics con-
tained in the formal expression for the dielectric response. Reference 26 is valid chiefly for the
intra-band transition while our paper is devoted to the interband transition, particularly the
hybridization effect of the hole band. Sec. III is devoted to a quantum many-body descrip-
tion for the medium polarization in a QW, in which the hybridization for the heavy hole
subband and the light hole subband is emphasized. Although the complex valence band in a
QW and the related exciton problem has been widely treated in the literatures, a complete
treatment that starts from the quantum many-body theory for the QW exciton, and includes
non-local response function and complete symmetry analysis for the 4-component spinor like
wavefunction, is still absent. We shall present such a complete and detailed treatment in this
section. In Sec. III-A, we give an expression for the medium polarization propagator with
both positive and negative frequency parts, which is applicable to generic non-translational
invariant systems. In Sec. III-B, by summing over the Kramer’s degenerate states, we show
the detailed expression for the nonlocal conductivity tensor which is proved to be diagonal
and can be factorized into a sum of bi-products. This makes its non-locality effect explicit. In
Sec.IV we present the final complete set of self-consistent equations as well as the boundary
conditions which are put into a discrete version for the convenience of practical calculation.
As an application, we discuss the ”selection rules” for the exciton-cavity coupling. Sec.V
gives some concluding remarks.

II. DESCRIPTION OF A QUANTUM WELL IN A CAVITY CONFINED BY
DISTRIBUTED BRAGG REFLECTORS.

The SMC under consideration consists of a QW of thickness Λ embedded in a thin layer
semiconductor material which is sandwiched between a pair of distributed Bragg reflectors.
This semiconductor layer serves as the barrier for the electrons and holes in the QW, while
it forms an optical cavity confined by the DBR’s. The whole structure is schematically
illustrated in Fig. 1. Although we only treat the case for one QW in the cavity, generalization to more complex cases can be easily done. The thickness of the cavity is $L_c$ with $\varepsilon_c(\omega)$ as its medium’s dielectric constant, where $\omega$ is the light radiation frequency. We assume that the QW medium has the same (background) dielectric constants as those of the cavity medium. The left (right) DBR is constructed from $N_L$ ($N_R$) pairs of two alternating layers. One of the two layers has a length $L_1$ and dielectric constant $\varepsilon_1(\omega)$ while the other $L_2$ and $\varepsilon_2(\omega)$, respectively. We choose the $z$-axis as the growth direction with $z = 0$ being the center of the system. Thus, the QW is located at $(-\Lambda_2, \Lambda_2)$ and the SMC occupies a region from $-L_c/2$ to $L_c/2$ with $L_c \geq \Lambda$. Consequently, $-L_c/2$ ($L_c/2$) is the boundary between the left (right) DBR and the SMC. Moreover, we rotate the coordinate axis around the $z$-axis in such a way to make the incident light propagate in the $x-z$ plane. Then the wave vector has the form $\vec{q} = (q_x \equiv q_\parallel, 0, q_z \equiv q_\perp)$ with $q_y$ being always equal to zero. As a result, for the $p$-polarized wave, the electric field has only $x-$ and $z-$ components, $E_x$ and $E_z$, respectively, while for the $s$-polarized wave the electric field has only a $y$-component $E_y$. For a propagating wave with fixed frequency and $\vec{q}_\parallel = q_\parallel \vec{e}_x$ (where $\vec{e}_\mu$, $\mu = x, y, z$ is the unit vector along the $\mu$-axis), its electric field has the form

$$\vec{E}(\vec{r}, t) = \vec{E}(\omega, \vec{q}_\parallel, z)e^{i(q_\parallel x - \omega t)} = \vec{E}(\omega, \vec{r})e^{-i\omega t}.$$  

The Maxwell equation for the electric field can be written as

$$\left[ \hat{I} \left( \nabla^2 + \frac{\omega^2}{c^2} \varepsilon_i(\omega) \right) - \nabla \nabla \right] \cdot \vec{E}(\omega, \vec{r}) = -\frac{4\pi i\omega}{c^2} \vec{j}(\omega, \vec{r})$$  

in which “$i$” is the medium index. Taking into consideration Eq.(2.1), Eq.(2.2) can be simplified to

$$\hat{L}_i(\omega, \vec{q}_\parallel) \cdot \vec{E}(\omega, \vec{q}_\parallel, z) = -\frac{4\pi i\omega}{c^2} \vec{j}(\omega, \vec{q}_\parallel z)$$  

with

$$\hat{L}_i(\omega, \vec{q}_\parallel) = \hat{I} \left( \frac{\partial^2}{\partial z^2} - q^2_\parallel \right) + \frac{\omega^2}{c^2} \varepsilon_i(\omega) - \left( i\vec{q}_\parallel + \vec{e}_z \frac{\partial}{\partial z} \right) \left( i\vec{q}_\parallel + \vec{e}_z \frac{\partial}{\partial z} \right).$$  

For simplicity, from now on we discuss mainly the $p$-polarized wave propagation. It is straightforward to convert the discussions for a $p$-polarized wave into those for an $s$-polarized wave. We will do this when necessary. Outside the QW medium, the polarization current
density $j(\omega, \vec{q}_i, z) = 0$ in Eq. (2.3). We then have plane wave solutions with

$$q_{\perp,i} = \left[ \frac{\omega^2}{c^2} \varepsilon_i(\omega) - q_{\parallel}^2 \right]^{1/2}$$

(2.5)

For the left DBR, denoting the $x$-components of the incident and reflected amplitudes of the electric field as $A_0$ and $B_0$, which are defined as approaching to and leaving from the right boundary of the left DBR. By applying the method of ref. 27, we obtain the corresponding electric field amplitude at the right boundary of the left DBR as $A_1$ and $B_1$, which are also defined by approaching the boundary from the left as

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \begin{pmatrix} T^L_{11} & T^L_{12} \\ T^L_{21} & T^L_{22} \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix}$$

(2.6)

with

$$\begin{pmatrix} T^L_{11} & T^L_{12} \\ T^L_{21} & T^L_{22} \end{pmatrix} = \begin{pmatrix} t^L_{11} & t^L_{12} \\ t^L_{21} & t^L_{22} \end{pmatrix}^{N_L}$$

(2.7)

where $T^L$ is the transfer matrix of the left BDR, $t^L$ is the transfer matrix of a pair of layers with different dielectric constants, as a unit cell of the left DBR, in the DBR and $N_L$ is the number of the pairs in the DBR. Then for the right DBR, we introduce further $A_3$ and $B_3$, the forward (along the $z$-direction) and backward (in the negative $z$ direction) amplitudes of the electric field, respectively. They are defined by approaching from the right to the left boundary of the right DBR. Meanwhile, $A_4$ and $B_4$ are the corresponding amplitudes at the right boundary of the right DBR which are also defined by approaching the boundary from the right. We can similarly define the transfer matrix by solving the homogeneous Maxwell equations 27 to obtain

$$\begin{pmatrix} A_3 \\ B_3 \end{pmatrix} = \begin{pmatrix} T^R_{11} & T^R_{12} \\ T^R_{21} & T^R_{22} \end{pmatrix} \begin{pmatrix} A_4 \\ B_4 \end{pmatrix}$$

(2.8)

with

$$\begin{pmatrix} T^R_{11} & T^R_{12} \\ T^R_{21} & T^R_{22} \end{pmatrix} = \begin{pmatrix} t^R_{11} & t^R_{12} \\ t^R_{21} & t^R_{22} \end{pmatrix}^{N_R}$$

(2.9)

The detailed expressions for the matrix elements $t^L_{i,j}$ and $t^R_{i,j}$ with $i, j = 1, 2$ are shown in Appendix A.

In the QW region, there is a sort of additional polarization effect of the medium other than that described by its background dielectric constant. This is because the virtual electron-hole pairs creation and annihilation processes will renormalize the light propagation
in the QW region. In particular, the Coulomb interaction between the virtual electron-hole pairs may play a crucial role in a certain frequency range. In this section, we just introduce formally a conductivity tensor \( \sigma(\omega, \vec{q}_\parallel; z, z') \) to describe this effect, such that

\[
\vec{j}(\omega, \vec{q}_\parallel, z) = \int d z' \vec{\sigma}(\omega, \vec{q}_\parallel; z, z') \cdot \vec{E}(\omega, \vec{q}_\parallel, z')
\] (2.10)

which will be further investigated in the next section. Therefore, in the SMC region (including the QW), the Maxwell equation (2.3) and (2.4) can be converted into an integral equation as

\[
\vec{E}(\omega, \vec{q}_\parallel; z) = \vec{E}^{(c)}(\omega, \vec{q}_\parallel; z) - \frac{4 \pi i}{c^2} \sum_{\nu} \int_{-\Lambda/2}^{\Lambda/2} dz' \int_{-\Lambda/2}^{\Lambda/2} dz'' G_x(\omega, \vec{q}_\parallel; z, z') \cdot \vec{\sigma}(\omega, \vec{q}_\parallel; z', z'') \cdot \vec{E}(\omega, \vec{q}_\parallel, z''')
\] (2.11)

in which

\[
\vec{E}^{(c)}(\omega, \vec{q}_\parallel; z) = (A_c e^{i q_{\perp} c z} + B_c e^{-i q_{\perp} c z}) \vec{e}_x - \frac{q_{\parallel}}{q_{\perp, c}} (A_c e^{i q_{\perp, c} z} - B_c e^{-i q_{\perp, c} z}) \vec{e}_z
\] (2.12)

is the homogeneous solution of Eq.(2.3), while \( G(\omega, \vec{q}_\parallel; z, z') \) is the Green’s function\(^{28}\) for the equation

\[
\vec{\xi}(\omega, \vec{q}_\parallel) \cdot \vec{\xi}(\omega, \vec{q}_\parallel; z, z') = \delta(z - z').
\] (2.13)

We can easily solve Eq.(2.13) up to a homogeneous solution of itself with its explicit expression shown in Appendix A. We notice that, in all equations, from Eq.(2.11) to Eq.(2.13), \( z \) and \( z' \) are confined to the region

\[
- \frac{L_c}{2} \leq z \leq \frac{L_c}{2}
\] (2.14)

Moreover, the integral equation (2.11) exhibits the nonlocality not only provided by the Green’s functions, but also induced by the medium polarization effect which is described by the conductivity tensor. To solve this integral equation, we emphasize that it should be solved with proper boundary conditions (BC’s). This is because neither the homogeneous solution \( \vec{E}^{(c)}(\omega, \vec{q}_\parallel, z) \) nor the Green’s functions are solved with respect to the correct BC’s for the SMC. Therefore, following classical electrodynamics, at \( z = \pm \frac{L_c}{2} \) we should have the BC

\[
A_1 + B_1 = A_c e^{-i q_{\perp, c} \frac{L_c}{2}} + B_c e^{i q_{\perp, c} \frac{L_c}{2}}
\]

\[
- \frac{4 \pi i}{c^2} \sum_{\nu'=x,z} \sum_{\nu''=x,z} \int_{-\Lambda/2}^{\Lambda/2} dz' \int_{-\Lambda/2}^{\Lambda/2} dz'' G_{x, \nu'}(\omega, \vec{q}_\parallel; -\frac{L_c}{2}, z')
\]
\[ \times \sigma_{\nu',\nu''}(\omega, \vec{q}_0; z', z'') E_{\nu''}(\omega, \vec{q}_0; z'') \]  

\[ \frac{\varepsilon_1}{q_{\perp, 1}} (A_1 - B_1) = \frac{\varepsilon_c}{q_{\perp, c}} (A_c e^{-i\nu_{\perp, 1} \frac{L_0}{2}} - B_c e^{i\nu_{\perp, 1} \frac{L_0}{2}}) \]

\[ + \frac{\varepsilon_c}{q_{\perp, c}} \frac{4\pi i\omega}{c^2} \sum_{\nu' = x,z} \sum_{\nu'' = x,z} \int_{-\Lambda/2}^{\Lambda/2} dz' \int_{-\Lambda/2}^{\Lambda/2} dz'' G_{x,\nu''}(\omega, \vec{q}_0; z', z'') \]

\[ \times \sigma_{\nu',\nu''}(\omega, \vec{q}_0; z', z'') E_{\nu''}(\omega, \vec{q}_0; z'') \]  

\[ \frac{\varepsilon_1}{q_{\perp, 1}} (A_3 - B_3) = \frac{\varepsilon_c}{q_{\perp, c}} (A_c e^{i\nu_{\perp, 1} \frac{L_0}{2}} - B_c e^{-i\nu_{\perp, 1} \frac{L_0}{2}}) \]

\[ - \frac{4\pi i\omega}{c^2} \sum_{\nu' = x,z} \sum_{\nu'' = x,z} \int_{-\Lambda/2}^{\Lambda/2} dz' \int_{-\Lambda/2}^{\Lambda/2} dz'' G_{x,\nu''}(\omega, \vec{q}_0; z', z'') \]

\[ \times \sigma_{\nu',\nu''}(\omega, \vec{q}_0; z', z'') E_{\nu''}(\omega, \vec{q}_0; z'') \]  

for fixed \( \omega \) and \( \vec{q}_0 \), since \( A_0 \) is the input while \( B_4 \) is usually taken to be zero. Here we have altogether eight independent constants \( B_0, A_1, B_1, A_c, B_c, A_3, B_3 \) and \( A_4 \), and a two-component electric field function \( E_x(\omega, \vec{q}_0, z) \) and \( E_z(\omega, \vec{q}_0, z) \) as unknown variables (functions), in which \( E_x \) and \( E_z \) are defined only in the SMC (including the QW). We stress that they are mutually coupled to each other through Eqs. (2.6), (2.8), (2.15)-(2.18) and the integral equation Eq.(2.11) (referring also to Eqs. (2.12) and (A1)-(A3)). Eqs. (2.6) and (2.8) are 2 \times 2 matrix equations, the above equations are exactly eight mutually coupled algebraic equations and a two-component integral equation, which solves self-consistently the whole DBR–SMC(QW)–DBR system as long as we have the detailed expression for the conductivity tensor. Such a description constitutes our mathematical framework for studying semiclassically the excitonic polaritons in the QW embedded in a SMC. The pair of DBR’s is coherently correlated with the SMC and plays the role of mode selection. Thus, the existing modes in the SMC not only dynamically couple to the semiconductor medium in the QW, but also coherently couple to the DBR’s. This is the physical meaning of such a description.
III. POLARIZATION OF THE SEMICONDUCTOR MEDIUM IN A QUANTUM WELL

In this section we concentrate on the polarization of the semiconductor medium in a quantum well. As mentioned in the introduction, the loss of displacement invariance in the growth direction of the QW and whole microstructure makes the dielectric function nonlocal. The non-locality of the medium polarization is closely related to the wave functions, and these functions are closely related to the band structure of the semiconductors. Thus, first of all, we should give a brief description of the band structure of the semiconductor microstructures. It is well known that the electronic states in a microstructure such as a QW can be satisfactorily described by the envelope function approximation. However, in many publications, this approximation is often an oversimplified version, i.e. the electron and holes are described as free particles with simple effective masses. Such a simplification usually works well in most cases, especially for conduction band electrons. However, this is not true for valence bands, i.e. for holes. The top of the valence bands of the semiconductors with $T_d$ symmetry belongs to the $\Gamma_8$ irreducible representation, which is 4-fold degenerate. In bulk material, the valence states apart from the $\Gamma$ point can be divided into heavy and light holes, both of which exhibit strong anisotropy and non-parabolicity. For the microstructure case such as in a QW, the situation is more complex. Generally speaking, any valence wavefunction can only be described by a four-component spinor, the basis of this spinor i.e. the Bloch cell periodic function (with spin) satisfies certain space transformation relations, and more importantly, for different components the envelope functions have different space rotational transformation properties. This invalidates the simple free particle picture. Although the problem of hole subband structure and related exciton’s as well as the optical transitions have been treated by several authors, the complete analysis based on the exact non-local dielectric function and four-spinor nature of the wave function is still absent. We will devote the following section to this problem.

For the usual III-V compound semiconductors, at the conduction band bottom $\Gamma_6$, the
Bloch cell periodic function \( u^{(0)}_{\alpha}(\vec{r}) \) is a spin doublet with index \( \alpha = \frac{1}{2}, -\frac{1}{2} \), while at the top of the valence band \( \Gamma_8 \) the cell function \( u^{(e)}_{\alpha'}(\vec{r}) \) can be regarded as a four component spinor with \( \alpha' = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2} \), the HH subband corresponding to \( \alpha' = \pm \frac{3}{2} \), and the LH subband to \( \alpha' = \pm \frac{1}{2} \). The plus and minus signs refer to time reversal (Kramer’s) degenerate states. In the effective mass approximation, the non-interacting Hamiltonian for the envelope functions written in the first quantization representation has the form

\[
H^{(0)}_{\alpha,\alpha';\beta,\beta'} = H^e_{\alpha,\beta} \delta_{\alpha',\beta'} + \delta_{\alpha,\beta} H^h_{\alpha',\beta'}
\]

\[
H^e_{\alpha,\beta} = \delta_{\alpha,\beta} \left[ \frac{1}{2m^e_{\|}} \left( \frac{\hbar}{i} \frac{\partial}{\partial r_{\|,e}} \right)^2 + \frac{1}{2m^e_{\perp}} \left( \frac{\hbar}{i} \frac{\partial}{\partial z_e} \right)^2 + E_g - \mu + V_e(\vec{r}_{\|,e}, z_e) \right]
\]

\[
H^h_{\alpha',\beta'} = \frac{1}{2m} \begin{pmatrix} P_1, & Q, & R, & 0 \\ Q^*, & P_2, & 0, & R \\ R^*, & 0, & P_2, & -Q \\ 0, & R^*, & Q, & P_1 \end{pmatrix} + \delta_{\alpha',\beta'}(\mu + V^h_{\alpha'}(\vec{r}_{\|,h}, z_h))
\]

where

\[
\begin{align*}
P_1 &= (\gamma_1 + \gamma_2) \left( \frac{\hbar}{i} \frac{\partial}{\partial r_{\|,e}} \right)^2 + (\gamma_1 - 2\gamma_2) \left( \frac{\hbar}{i} \frac{\partial}{\partial z_e} \right)^2 \\
P_2 &= (\gamma_1 - \gamma_2) \left( \frac{\hbar}{i} \frac{\partial}{\partial r_{\|,e}} \right)^2 + (\gamma_1 + 2\gamma_2) \left( \frac{\hbar}{i} \frac{\partial}{\partial z_e} \right)^2 \\
Q &= -i2\sqrt{3}\gamma_3 \left( \frac{\hbar}{i} \frac{\partial}{\partial x_e} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial x_h} \right) - i \left( \frac{\hbar}{i} \frac{\partial}{\partial y_h} \right) \\
R &= \sqrt{3} \gamma_2 \left( \frac{\hbar}{i} \frac{\partial}{\partial x_e} \right)^2 - \left( \frac{\hbar}{i} \frac{\partial}{\partial y_h} \right)^2 - 2i\gamma_3 \left( \frac{\hbar}{i} \frac{\partial}{\partial x_h} \right) \left( \frac{\hbar}{i} \frac{\partial}{\partial y_h} \right)
\end{align*}
\]

In Eqs. (3.2)-(3.4), the conduction electron coordinate is giving by \( \vec{r}_e = (\vec{r}_{\|,e}, z_e) \) with \( \vec{r}_{\|,e} = x_e \vec{e}_x + y_e \vec{e}_y \), and the valence hole coordinate by \( \vec{r}_h = (\vec{r}_{\|,h}, z_h) \) with \( \vec{r}_{\|,h} = x_h \vec{e}_x + y_h \vec{e}_y \); \( E_g \) is the gap which separates the conduction band and the valence band, \( \mu \) the chemical potential, \( m \) the physical electron mass, and \( m^e_{\perp} \) and \( m^e_{\|} \) are effective masses of the conduction electrons corresponding to motion perpendicular or parallel to the \( z \)-axis; \( V^e \) and \( V^h \) are the confinement potentials which form the barriers for the QW. For the DBR–SMC(QW)–DBR system discussed in this paper, \( V_e \) and \( V_h \) are actually \( \vec{r}_{\|,e} \) and \( \vec{r}_{\|,h} \) independent. Eq.(3.3) with (3.4) is the well known Luttinger Hamiltonian which is written down in a form with a specific choice of the coordinates. In these two equations, \( Q \) and \( R \) describe the hybridization between the HH and LH subbands, while \( \gamma_1, \gamma_2 \) and \( \gamma_3 \) are band structure parameters.
We notice that the envelope function description adopted in this paper is valid around the $\Gamma$ point. We denote $\varphi_{b,\lambda}(\vec{r})$ as the envelope function which can be solved from the eigenvalue equation for the Hamiltonian equations (3.2) and (3.3) with appropriate boundary conditions in connection with the confinement barriers. Its corresponding energy eigenvalue is denoted by $\varepsilon_{s}^{(b,\lambda)}$. In this notation, $b = c$ refers to the conduction band with $\lambda = \pm \frac{1}{2}$ corresponding to a spin doublet; $b = v$ refers to the valence band with indices $\lambda = \pm \frac{3}{2}$, $\pm \frac{1}{2}$ which describe valence band branches resulting from diagonalization of the hybridized Hamiltonian Eq. (3.3). Notice that each of the eigenfunctions (envelope functions) corresponding to these branches is a four component spinor. We again name the envelope functions with $\lambda = \pm \frac{3}{2}$ as the HH branch and that with $\lambda = \pm \frac{1}{2}$ as the LH branch, according to the properties that the $\lambda$-spinor has the dominant component as $\alpha = \lambda$. Moreover, $s$ is the quantum number depending on the confinement potential. It is discrete along the direction of confinement but continuous in the extended directions.

A. Semiconductor Medium Polarization Induced by Virtual Electron-Hole Pairs

It is known that the conductivity tensor is connected to the medium’s polarization tensor by

$$\sigma(\omega; \vec{r}, \vec{r}^\prime) = \frac{i}{\omega} \varepsilon_r(\omega; \vec{r}, \vec{r}^\prime)$$

Intuitively, during light propagation, the dominant contribution to the medium’s polarization should be the virtual excitations of electron-hole pairs. To clarify certain conceptual problems we shall discuss the ideal situation: the intrinsic state of the QW at low temperature, i.e., the valence band is almost fully filled while the conduction band is almost completely empty. The virtual pairs thus consists of conduction electrons and valence holes. In such a case, the Coulomb interaction should induce a series of exciton states distributed in the semiconductor gap. These are bound states formed by conduction electrons and valence holes. These virtual bounded $e - h$ pairs should also contribute to the medium’s polarization even at zero temperature for an intrinsic QW. Based upon such an understanding, the
polarization can be calculated straightforwardly as outlined in Appendix B. We notice that there are no requirements for the spatial translational invariance, so that it can be applied to any sort of QW. This also has the advantage that when applied to the planar QW, the in-plane center of mass momentum for the excitons can be explicitly treated, which is a non-trivial property for the excitonic polaritons. Now, the derived expression has the form
\[
\frac{\mathcal{H}}{2\gamma}(\omega; \vec{r}, \vec{r}') = \left( \frac{\hbar}{m} \right)^2 \sum_{\alpha} \sum_{\alpha'} \sum_{\beta} \sum_{\beta'} \sum_{\gamma} \langle v, \alpha' | \vec{p} | c, \alpha \rangle \langle c, \beta | \vec{p} | v, \alpha \rangle 
\times \left\{ \frac{\psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}, \vec{r}') \psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}, \vec{r}')}{\omega + i\eta - E_n^{(\lambda, s; \lambda', s'; n)}} - \frac{\psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}, \vec{r}') \psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}, \vec{r}')}{\omega + i\eta + E_n^{(\lambda, s; \lambda', s'; n)}} \right\},
\]
(3.6)
in which
\[
\psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}, \vec{r}') = \psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}_h, \vec{r}_h)|_{\vec{r}_e = \vec{r}_h = \vec{r}},
\]
(3.7)
where \(\psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}_e, \vec{r}_h)\) is the two body exciton-like wave function for the \(n\)-th eigenstate which consists of a conduction electron with quantum numbers \(\lambda, s\) in \((\vec{r}_e, \alpha)\) representation and a valence hole with quantum numbers \(\lambda'\) and \(s'\) in the \((\vec{r}_h, \alpha')\) representation. It satisfies
\[
\sum_{\beta, \beta'} \left( H_{\alpha, \alpha'; \beta, \beta'}^{(0)} - \delta_{\alpha, \beta} \delta_{\alpha', \beta'} \frac{\hbar^2}{2\varepsilon_{\vec{r}_e - \vec{r}_h}} \right) \psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}_e, \vec{r}_h) = E_n^{(\lambda, s; \lambda', s')} \psi^{(\lambda, s; \lambda', s'; n)}(\vec{r}_e, \vec{r}_h),
\]
(3.8)
where the eigenvalue \(E_n^{(\lambda, s; \lambda', s')}\) is exactly the energy term appearing in Eq.(3.6). In Eq.(3.8), we have also introduced the dipole matrix element
\[
\langle c, \alpha | \vec{p} | v, \alpha' \rangle \equiv \frac{1}{\Omega} \int_{\Omega} d^3\vec{r} \frac{\hbar}{2\varepsilon}(u^{(c)}_{\alpha}(\vec{r}) \nabla u^{(v)}_{\alpha'}(\vec{r}) - \nabla u^{(c)}_{\alpha'}(\vec{r}) \cdot u^{(v)}_{\alpha}(\vec{r})),
\]
(3.9)
where \(\Omega\) is the volume of the crystal cell and the integration is also confined within the cell. We emphasize here that, for the inter-band processes, the dipole matrix element is carried by the Bloch cell functions but not by the envelope functions. In Eq.(3.8) only the two-body wave functions with its arguments \(\vec{r}_e = \vec{r}_h = \vec{r}\) contribute to the spectral weight of polarization propagator, \(\vec{r}\) is the point where the electron meets the hole. Moreover, the first term in the bracket of Eq. (3.9) is its positive frequency part while the second is the negative frequency part. Both parts are necessary for a boson-like propagator. We notice that the \(\vec{r}\) and \(\vec{r}'\) change into each other in the two corresponding spectral weights, for which we understand that the positive and negative frequency parts correspond to a sort of
forward and backward propagation, respectively. Only when a certain kind of symmetry is present for the system under investigation will the two spectral weight functions be equal to each other. This is one of the main topics for the next sub-section.

We notice that the extended eigenstates of Eq.(3.8) can also contribute to the spectral function. Since they are off-resonance from our interested frequencies, their contribution has been included in the background dielectric constants.

B. Summation over the Degenerate States Based on Space-Time Inversion Symmetries

After performing a summation over the space-time reversal transformation connected degenerate states, we show in this subsection that not only the positive and negative frequency parts in the polarization propagator can be combined into one term, but also the non-diagonal elements for the polarization tensor can diminish. This will make the expression neat and further simplifies the calculation a great deal.

We apply the formal discussion in the previous sub-section to the system we interested in - a planar QW embedded in a DBR-SMC-DBR system (see Sec. II). The general subband indices and quantum numbers $\lambda, s; \lambda', s'$ and $n$ are now specified into the following symbols: $\vec{q}_\parallel; n_{ex}, l; n, j_c; n', j_h$. Here $\vec{q}_\parallel$ is the 2D center of mass momentum for the exciton, which is a good quantum number describing the translational invariance in the $X$-$Y$ plane for the system; $n_{ex}$ and $l$ are the quantum numbers for the eigenstate of the exciton describing the in-plane relative motion for the virtual electron and hole pairs; $n_{ex}$ is the major quantum number while $l$ is the angular quantum number; $n$ ($n'$) is the index of the discrete states due to the confinement in the $z$-direction of the conduction electrons (valence holes); $j_c = \pm \frac{1}{2}$ are the subband indices describing the spin doublet for the conduction electrons while $j_h = \pm \frac{1}{2}, \pm \frac{3}{2}$ are the subband indices for the valence holes representing the total angular momentum induced by spin-orbit coupling.

To solve $\psi_{\alpha, \alpha'}^{(\vec{q}_\parallel; n_{ex}, l; n, j_c; n', j_h)}(\vec{r}_e, \vec{r}_h)$ from Eq.(3.8) we need the complete set of eigenfunctions.
of the non-interacting Hamiltonian described by Eqs (3.2) and (3.3) for the conduction electrons and valence holes, respectively. These are

\[
\frac{1}{\sqrt{L^2}} e^{i\vec{k}_\parallel \cdot \vec{r}_\parallel} \varphi_n^{(e)}(z_e) \delta_{j_e,\alpha}
\]

for the conduction electrons and

\[
\frac{1}{\sqrt{L^2}} e^{i\vec{k}_\parallel \cdot \vec{r}_\parallel} \varphi_n^{(v)}(\vec{k}_{||h}, z_h)
\]

for the valence holes with subband hybridization, where \( L^2 \) is the extension for the QW in the \( X-Y \) plane. In solving Eqs. (3.2) and (3.3), there is an energy eigenvalue \( \epsilon_n^{(e)} \) associated with \( \varphi_n^{(e)}(z_e) \) for the \( z \)-direction electronic motion and another eigenvalue \( \epsilon_n^{(v)}(\vec{k}_{||h}, z_h) = \epsilon_n^{(v)}(\vec{k}_{||h} = 0) \) associated with \( \varphi_n^{(v)}(\vec{k}_{||h}, z_h) \) which could also be interpreted as describing the \( z \)-direction hole motion. Actually, for a hole in the valence band, its motion along the \( z \)-direction described by the eigen wave function \( \varphi_n^{(v)}(\vec{k}_{||h}, z_h) \) is coupled to its motion in the \( X-Y \) plane characterized by \( \vec{k}_{||h} \). So \( \varphi_n^{(v)}(\vec{k}_{||h}, z_h) \) depends not only on \( z_h \) but also on \( \vec{k}_{||h} \) whilst \( \epsilon_n^{(v)}(\vec{k}_{||h}) \) also has the \( \vec{k}_{||h} \) dependence. Such a subtlety is due to the hybridization term \( Q \) and \( R \) in Eq. (3.3) and (3.4).

We notice further that, in the QW region, \( V_h^{(\alpha')}(\vec{r}_{||h}, z) \) is constant so that we choose it to be zero. The \( z \)-axis parities of the matrix elements of the Luttinger Hamiltonian Eq. (3.3) change their signs alternately along each row and each column. This interesting symmetry property makes the hole eigenfunction for Eq. (3.3) have an amazing parity symmetry so that the first and third components \( (\alpha' = \frac{3}{2}, -\frac{1}{2}) \) have the same parity symmetry along the \( z \)-axis which is opposite to that of the other two components \( (\alpha' = \frac{1}{2}, -\frac{3}{2}) \). Moreover, since the Luttinger parameters \( \gamma_2 \) and \( \gamma_3 \) are usually rather close to each other, we may assume that they are equal, i.e. \( \gamma_2 = \gamma_3 \). We further introduce a polar coordinate \( (k_{||h}, \vartheta_h) \) for \( \vec{k}_{||h} \) in the \( X-Y \) plane, \( k_{||h} = k_{||h}(\cos \vartheta_h \vec{e}_x + \sin \vartheta_h \vec{e}_y) \). Following Eq. (3.4), we have \( Q \sim e^{-i\vartheta_h} \) and \( R \sim e^{-2i\vartheta_h} \). As a result, the corresponding eigenfunction in Eq. (3.11) acquires the following functional dependence

\[
\varphi_n^{(v)}(\vec{k}_{||h}, z_h) = e^{i(\vartheta_h - \alpha') \vartheta_h} \varphi_n^{(v)}(\vec{k}_{||h}, z_h)
\]

in which \( \vartheta_h \) is separated from \( \varphi_n^{(v)}(\vec{k}_{||h}, z_h) \) and the product \( k_{||h}z_h \) is a single dimensionless
We then expand the two-body exciton-like wave function in terms of the non-interacting electron and hole wave functions, Eqs. (3.10) and (3.11) for a fixed set of good quantum numbers $\vec{q}_{||}; n_{ex}, l; n, j_e; n', j_h$, and obtain

$$
\psi^{(q_{||}; l; n_{ex}, l; n, j_e; n', j_h)}(\vec{r}_e, \vec{r}_h) = \frac{1}{L} \sum_{\vec{k}_{||}, e} \sum_{\vec{k}_{||}, h} \delta_{\vec{q}_{||}, \vec{k}_{||}, e + \vec{k}_{||}, h} \delta_{\vec{q}_{||}, \vec{k}_{||}, e + \vec{k}_{||}, h} e^{i(\vec{k}_{||}, e - \vec{q}_{||}, e + \vec{k}_{||}, h - \vec{q}_{||}, h)}.
$$

The expansion coefficient $f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}, e, \vec{k}_{||}, h)$ can be understood as the 2D excitonic wave function for which the center of mass degree of freedom has been separated. If we ignore the hybridization terms $Q$ and $R$ in the hole Hamiltonian Eq. (3.3), and further ignore the $z_e$ and $z_h$ dependence for the Coulomb interaction in Eq. (3.8) because the thickness of the QW is rather small, we can show easily that $f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}, e, \vec{k}_{||}, h)$ would be precisely the 2D hydrogen atom solution of Eq. (3.8) constrained by $\vec{q}_{||} = \vec{k}_{||}, e + \vec{k}_{||}, h$. Since now we have the hybridization, the physical meaning of $f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}, e, \vec{k}_{||}, h)$ is no longer so transparent, and the coefficient should be determined by substituting itself into Eq. (3.8). Actually we need only the value of the wave function (3.13) at $\vec{r}_e = \vec{r}_h = \vec{r}$. Thus, we have

$$
\psi^{(q_{||}; l; n_{ex}, l; n, j_e; n', j_h)}(\vec{r}, \vec{r}) = \frac{1}{\sqrt{L^2}} e^{i\vec{q}_{||}, \vec{r}_h} \delta_{j_e, \alpha} \frac{1}{L^2} \sum_{\vec{k}_{||}, e} \sum_{\vec{k}_{||}, h} \delta_{\vec{q}_{||}, \vec{k}_{||}, e + \vec{k}_{||}, h} f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}, e, \vec{k}_{||}, h) \phi^{(c)}_{n}(z) \phi^{(v)}_{n', j_h, \alpha}(\vec{k}_{||}, h, z)
$$

Moreover, the GaAs system has an energy gap $\sim 1.5$ eV. The wavelength of interest has an order of magnitude $\sim 10^3$ Å. On the other hand, the effective Bohr radius for the 2D-exciton in GaAs has the order of magnitude $\sim 10^2$ Å. Therefore, $\vec{k}_{||}, e$ and $\vec{k}_{||}, h$ will span a region in momentum space in which the 2D excitonic wave function $f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}, e, \vec{k}_{||}, h)$ has non-negligible contributions, much bigger than that of $\vec{q}_{||}$. We may reasonably set $\vec{q}_{||}$ to be $\sim 0$ in the double summation for $\vec{k}_{||}, e$ and $\vec{k}_{||}, h$, i.e., we may have approximately $\vec{k}_{||}, h \simeq -\vec{k}_{||}, e = \vec{k}_{||}$ in Eq. (3.14) within the double summation. Then

$$
\psi^{(q_{||}; l; n_{ex}, l; n, j_e; n', j_h)}(\vec{r}, \vec{r}) = \frac{1}{\sqrt{L^2}} e^{i\vec{q}_{||}, \vec{r}_h} \delta_{j_e, \alpha} \int \frac{d\vec{k}_{||}}{(2\pi)^2} f^{(n_{ex}, l)}_{n_{ex}, l}(\vec{k}_{||}) \phi^{(c)}_{n}(z) \phi^{(v)}_{n', j_h, \alpha}(\vec{k}_{||}, h, z).
$$

Intuitively, the 2D exciton-like wave function should have the expression
reversal symmetry property for the hole wave function has been introduced in connection with Eqs. (3.10) and (3.11). As mentioned above, due to the symmetry properties for the system which are exact. Due to the space-time reversal symmetry, $E_{ex, l}^{(n, n', j_h)}(q_{||})$ and $f_{ex, l}^{(n, n', j_h)}(k_{||})$ are degenerate with respect to $\pm l$, $j_c = \pm \frac{1}{2}$, $j_h = \pm \frac{1}{2}$ and $j_h = \pm \frac{3}{2}$. We have also the time reversal symmetry property for the hole wave function

$$\varphi^{(v)}_{n', j_h; \alpha'}(z) = \varphi^{(v)}_{n', -j_h; -\alpha'}(z).$$

Furthermore, all the $f_{ex, l}^{(n, n', j_h)}(k_{||})$, $\varphi^{(c)}_{n}(z)$ and $\varphi^{(v)}_{n, j_h; \alpha}(k_{||} z)$ are real functions. On the other
hand, it is known that there is only one independent matrix element for \( \langle v, \alpha' | p_\mu | c, \alpha \rangle \), i.e. 
\( p = \langle X | p_x | s \rangle = \langle Y | p_y | s \rangle = \langle Z | p_z | s \rangle \) where \( \langle X \rangle \), \( \langle Y \rangle \) and \( \langle Z \rangle \) are the orbital part of the Bloch cell functions for the hole band with \( l = 1 \) and \( |s\rangle \) is the orbital part of the Bloch cell functions for the conduction band. By making use of the Kramer’s degeneracy properties and the Clebsch-Gordon coefficients for the matrix elements \( \langle v, \alpha' | p_\mu | c, \alpha \rangle \), we can sum over the plus and minus values of \( l, j_z \) and \( j_h \) but keep the absolute values of \( l, j_c, j_h \) and the corresponding energy eigenvalue fixed. After a lengthy calculation, the conductivity tensor associated with Eqs. (3.3) and (3.18) can be derived in a diagonal form as

\[
\sigma_{\mu\nu}(\omega; \vec{r}, \vec{r}') = \frac{1}{L^2} \sum_{\vec{q}_\parallel} e^{i\vec{q}_\parallel \cdot (\vec{r}_\parallel - \vec{r}'_\parallel)} \sigma_{\mu\nu}(\omega; \vec{q}_\parallel; z, z')
\]

with

\[
\sigma_{\mu\nu}(\omega; \vec{q}_\parallel; z, z') = \frac{i \sqrt{2} \alpha^2}{\omega} \delta_{\mu\nu} \sum_{n} \sum_{n'j_h} \sum_{n_{ex},l} \sum_{l_h} P^{(n,n',j_h)}_{n_{ex},l}(\omega, q) \cdot \phi^{(n,n',j_h)}_{n_{ex},l}(z) \eta_{l}\phi^{(n,n',j_h)}_{n_{ex},l}(z'),
\]

in which

\[
\phi^{(n,n',j_h)}_{n_{ex},l}(z') = \int_{0}^{\infty} \frac{k_{||}dk_{||}}{2\pi} f^{(n,n',j_h)}_{n_{ex},l}(k_{||}) \varphi^{(v)}(z) \varphi^{(v)}(z')
\]

\[
P^{(n,n',j_h)}_{n_{ex},l} = \frac{2E^{(n,n',j_h)}_{n_{ex},l}(q)}{(\omega + i\gamma_{n_{ex},l}^{(n,n',j_h)}q_{||})^2 - [E^{(n,n',j_h)}_{n_{ex},l}(q_{||})]^2}.
\]

In Eqs. (3.22), (3.23) and (3.24), \( j_h \) takes the value of \( \frac{3}{2} \) and \( \frac{1}{2} \) for HH and LH bands, respectively, while \( l \) is equal to 0 and 1, \( h = 0 \) if \( l = 0 \), and \( h \) should be summed over \( \pm 1 \) if \( l = 1 \). This “new” quantum number \( h \) results from the summation over the degenerate states due to Kramer’s and space inversion symmetries. The term \( \eta_{l}^{(j_{h}^{d},j_{h}^{d})} \) comes from the Clebsch-Gordon coefficients for the dipole matrix elements, with

\[
\begin{align*}
\eta_{l}^{(3/2,0,0)} &= \eta_{l}^{(1/2,1,1)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
\eta_{l}^{(1/2,0,0)} &= \eta_{l}^{(3/2,1,1)} = \eta_{l}^{(1/2,1,-1)} = \begin{pmatrix} \frac{3}{4} \\ \frac{1}{4} \end{pmatrix} \\
\eta_{l}^{(3/2,1,1)} &= 0.
\end{align*}
\]

We stress that if we ignore the hybridization between the HH and LH subbands, then only \( l = 0 \) exciton states contribute to the spectral weight function. Meanwhile, \( \varphi^{(v)}_{n',j_h,j'=j_h}(k_{||}z) \) becomes \( \varphi^{(v)}_{n',j_h,j'=j_h}(z) \) which is independent of \( k_{||} \). Therefore, the hole subband hybridization
induced excitonic polaritons are characterized by the angular quantum number $l \neq 0$. We stress further that, in Eqs. (3.22) and (3.24), we replace $\omega + i\eta$ by $\omega + i\gamma_{n_{ex},l}$ in which $\gamma_{n_{ex},l}$ are the only phenomenological parameters introduced in this approach for describing the width of the exciton level.

IV. DISCRETE REPRESENTATION OF ELECTRIC FIELD IN AN SMC

In the last section, we obtained the polarization of a medium induced by the Coulomb interacting virtual electron-hole pairs in an intrinsic semiconductor QW at zero temperature. We notice that the $z, z'$ dependence for the conductivity tensor Eq.(3.22) is separated into a bi-product of two $\phi$-functions. Thus, the kernel of the integral in equation (2.11) is separable. Following Ref. 26, we can easily transform the integral equation (2.11) for the electric field in an SMC into an algebraic equation which could further simplify the calculations. In particular, as $P_{n_{ex},l}^{(n,n',j_h)}(\omega, q_l)$ has a resonant pole, only very few discrete components for the electric field are needed, and possibly only one may be sufficient.

Introducing

$$\vec{E}_{n_{ex},l}^{(n,n',j_h)}(\omega, q_l) = \int_{-\Lambda/2}^{\Lambda/2} dz \phi_{n_{ex},l}^{(n,n',j_h)}(z) \vec{E}(\omega, q_l; z),$$  (4.1)

we may express the electric field in terms of $\vec{E}_{n_{ex},l}^{(n,n',j_h)}(\omega, q_l)$ as

$$\vec{E}(\omega, q_l; z) = \vec{E}(\omega, q_l; z) + \frac{4\pi e^2}{m^* c^2} \times$$

$$\sum_{n,n',j_h} \sum_{n_{ex},l} \int_{-\Lambda/2}^{\Lambda/2} dz' P_{n_{ex},l}^{(n,n',j_h)}(\omega, q_l) G^{(n,n',j_h)}(\omega, q_l; z, z')$$

$$(\phi_{n_{ex},l}^{(n,n',j_h)}(z) \cdot \vec{F}_{n_{ex},l}^{(n,n',j_h)}(\omega, q_l)).$$  (4.2)

with

$$\eta^{(j_h,l,l_h)} = \delta_{\mu\nu} \eta_{(j_h,l,l_h)}^{(j_h,l,l_h)}.$$  (4.3)

We emphasize that the $\vec{F}$-functions introduced by Eq.(4.1) depend on the electric field defined only in the region of $[-\Lambda/2, \Lambda/2]$, but the corresponding electric field Eq.(4.2) is meaningful for the whole region of $[-Lc^2, Lc^2]$. Utilizing the above two equations, we can express Eq.(2.11) as well as the boundary condition Eqs. (2.15)-(2.18) in terms of $\vec{F}$-functions. We perform
the operation \( f'_{\text{DBR-SMC(QW)-DBR}} \) on both sides of Eq. (4.11), and introduce \( \tilde{f}(\omega, \vec{q}_||) = f'_{\text{DBR-SMC(QW)-DBR}} \) and \( \tilde{G}(\omega, \vec{q}_||) = \int_{-\Lambda/2}^{\Lambda/2} dz \phi^{s(n''n'''j_h)}(z) \tilde{E}(\omega, \vec{q}_||; z) \) (4.14)

\[
\phi^{s(n''n'''j_h)}(z) \tilde{E}(\omega, \vec{q}_||; z) = f'_{\text{DBR-SMC(QW)-DBR}}(z) \tilde{E}(\omega, \vec{q}_||; z)
\]

from which we obtain

\[
\tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||) = \int_{-\Lambda/2}^{\Lambda/2} dz \phi^{s(n''n'''j_h)}(z) \tilde{E}(\omega, \vec{q}_||; z) + \frac{4\pi e^2 p^2}{m e^2} \sum_{n''n'''j_h} \frac{\phi^{s(n''n'''j_h)}(z') \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||; z')}{z'}
\]

(4.15)

The boundary condition Eqs. (2.18) can also be reformulated in terms of \( F_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)} \) as

\[ A_1 + B_1 = A_c e^{i q_{\perp,L} L_c/2} + B_c e^{i q_{\perp,L} L_c/2} + \frac{4\pi e^2 p^2}{m e^2} \sum_{n''n'''j_h} \frac{\phi^{s(n''n'''j_h)}(z') \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||; z')}{z'}
\]

(4.16)

\[
\frac{\varepsilon_1}{\varepsilon_{q_{\perp,L}}} (A_1 - B_1) = \frac{\varepsilon_c}{\varepsilon_{q_{\perp,L}}} (A_c e^{-i q_{\perp,L} L_c/2} - B_c e^{i q_{\perp,L} L_c/2}) - \frac{\varepsilon_c}{\varepsilon_{q_{\perp,L}}} \frac{4\pi e^2 p^2}{m e^2} \sum_{n''n'''j_h} \frac{\phi^{s(n''n'''j_h)}(z') \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||; z')}{z'}
\]

(4.17)

\[
A_3 + B_3 = A_c e^{i q_{\perp,L} L_c/2} + B_c e^{-i q_{\perp,L} L_c/2} + \frac{4\pi e^2 p^2}{m e^2} \sum_{n''n'''j_h} \frac{\phi^{s(n''n'''j_h)}(z') \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||; z')}{z'}
\]

(4.18)

\[
\frac{\varepsilon_1}{\varepsilon_{q_{\perp,L}}} (A_3 - B_3) = \frac{\varepsilon_c}{\varepsilon_{q_{\perp,L}}} (A_c e^{i q_{\perp,L} L_c/2} + B_c e^{-i q_{\perp,L} L_c/2}) + \frac{\varepsilon_c}{\varepsilon_{q_{\perp,L}}} \frac{4\pi e^2 p^2}{m e^2} \sum_{n''n'''j_h} \frac{\phi^{s(n''n'''j_h)}(z') \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||; z')}{z'}
\]

(4.19)

Then, in terms of the discrete representation for the electric field \( \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||) \), the complete description of the DBR-SMC(QW)-DBR system is now given by Eqs. (4.8)-(4.11) and (4.3), referring also to Eqs. (2.6), (2.8), (2.12), (A3), (4.1), (4.2) and (4.13). Note that in order to express \( \tilde{F}_{n_{\text{DBR-SMC(QW)-DBR}}}^{(n''n'''j_h)}(\omega, \vec{q}_||) \) in Eq. (4.10) in terms of \( A_c \) and \( B_c \) we need to introduce two more
The terms \( w^{(n,n',j_h)}_{\text{ex},d_h}(\omega, \vec{q}_\parallel) \) and \( w'_{\text{ex},d_h}(\omega, \vec{q}_\parallel) \)
\begin{align*}
w^{(n,n',j_h)}_{\text{ex},d_h}(\omega, \vec{q}_\parallel) &= \int_{-\Lambda/2}^{\Lambda/2} dz e^{i q_{\perp,z,c}z} \phi_{\text{ex},d_h}^{s(n,n',j_h)}(z) \vec{E}(c)(\omega, \vec{q}_\parallel; z) \\
w'_{\text{ex},d_h}(\omega, \vec{q}_\parallel) &= \int_{-\Lambda/2}^{\Lambda/2} dz e^{-i q_{\perp,z,c}z} \phi_{\text{ex},d_h}^{*}(n,n',j_h)(z) \vec{E}(c)(\omega, \vec{q}_\parallel; z)
\end{align*}
(4.12)
according to Eq 2.12. Up to now, it is clear that we do not need the effective photon-exciton coupling constant any more in the approach we have adopted.

We have now established a complete set of equations which can give us the real space electric field distribution within SMC with non-local dielectric response of QW excitons embedded in it, and thus enable us to obtain various semiclassical optical properties. Compared with previous theoretical work, our approach treats both the electro-magnetic field and the electron excitation exactly and does not depend on any artificial parameters. Moreover, certain effects not considered in previous studies such as violation of simple selection rules and the strange angle dependence of the reflection spectrum, can be easily calculated using this approach. We will report these results elsewhere. As an application, we analyze some interesting aspects of the exciton "selection rule" for a symmetric microcavity.

It is well known from ordinary exciton models that only the \( S \) exciton can couple to the electromagnetic field, but due to the four component nature of the hole subband wave function and the existence of band mixing, the \( p \) exciton can also couple to the photon field and thus form polaritons in a microcavity. We call this a hybridization-induced exciton-polariton, and analyze the relevant parity propeties along the \( z \)-axis.

It can be seen that Eq. (4.12) in conjunction with expressions (3.23) and (4.1) shows explicitly how the non-locality for the conductivity behaves. Each term of the spectral weight function has the form of a product of two \( \phi \)-functions with one of the two depending only on \( z \) and the other on \( z' \). Therefore, one of them is convoluted with the electric field and plays a role as a “weight” function while the other is convoluted with the Green’s function as a “source” function, which strongly influences the effective coupling between light and the exciton. This makes the role of the parity symmetry along the \( z \)-axis explicitly important. Here we restrict ourself to the case of normal incidence and symmetric DBR pairs only.
As we have discussed in Sec. II-B, \( \varphi_n^{(c)}(z) \) and \( \varphi_{n,j_h,\alpha'}^{(v)}(k\parallel z) \) can be classified by the parity symmetry (along \( z \)-axis). In fact, the parity symmetry for the contributive component of the hole spinor wave functions is controlled by its index \( \alpha' = j_h + l_h \). Moreover, for an SMC confined by a pair of symmetric DBR’s, it is known that \( \vec{E}^{(c)}(\omega, \vec{q}\parallel; z) \) as a function of \( z \) is also an eigenstate of the parity symmetry at the resonant condition \( L_c = n\lambda/2 \), with \( n = 1, 2, \cdots \). By considering Eqs. (2.11), (A3), (3.22) and (3.23), we can verify that the electric field \( \vec{E}(\omega, \vec{q}\parallel; z) \) will have the same even-oddness as that of \( \vec{E}^{(c)}(\omega, \vec{q}\parallel; z) \). Following Eqs. (1.2), (2.4) and (3.23), the physics contributed by the QW depends strongly on the integral

\[
I^{(n,n',j_h)}_{l_h}(\omega, \vec{q}\parallel; k\parallel) = \int_{-\Lambda/2}^{\Lambda/2} dz \varphi_n^{(c)}(z) \varphi_{n',j_h,\alpha'}^{(v)}(k\parallel z) E_x(\omega, \vec{q}\parallel; z), \tag{4.13}
\]

and we can now find interesting consequences for the polaritons. If we set \( \varphi_n^{(c)}(z) \) for the conduction electron to be always in the \( n = 1 \) state, it will not contribute to the parity symmetry since it is an even function of \( z \). For a symmetric SMC, \( E^{(c)}(\omega, \vec{q}\parallel; z) \) is even for \( L_c = \lambda/2 \) and odd for \( L_c = \lambda \). Hence for an SMC of \( L_c = \lambda/2 \), the electric field is even. Then, following Eq.(3.17), only polaritons with quantum number \( l = l_h = 0 \) and the index \( \alpha' = j_h \) can survive in the SMC for both \( j_h = 1/2 \) and \( j_h = \frac{3}{2} \). This is because \( \varphi_{n' = 1,j_h,\alpha' = j_h}^{(v)}(k\parallel z) \) is an even function of \( z \). The hybridization induced polaritons with quantum number \( l = 1 \) cannot be observed since \( \varphi_{n' = 1,j_h,\alpha' = j_h \pm 1}^{(v)}(k\parallel z) \) are odd functions of \( z \) which will make \( I^{(1,1,j_h)}_{l_h = \pm 1}(\omega, \vec{q}\parallel; k\parallel) = 0 \). On the contrary, if we have an SMC of \( L_c = \lambda \), the electric field \( E_x(\omega, \vec{q}\parallel; z) \) becomes an odd function of \( z \), if \( \varphi_{n' = 1,j_h,\alpha' = j_h}^{(v)}(k\parallel z) \) is still an even function, the polaritons with quantum number \( n = n' = 1 \), \( l = 0 \) will be forbidden for the \( \lambda \)-SMC which will make \( I^{(1,1,j_h)}_{l_h}(\omega, \vec{q}\parallel; k\parallel) = 0 \). In this case, only the hybridization induced polariton can survive in the SMC since \( \varphi_{n' = 1,j_h,\alpha' = j_h \pm l_h}^{(v)}(k\parallel z) \) is odd. What we learned from the above discussion is that the even-oddness of the electric field depends on the cavity resonance condition, while the parity of the components of the electron or hole wave function depends only on the QW. Then we can have an interplay of the even-odd symmetry for the integrand of Eq.(1.1). As a result the parity symmetry along the \( z \)-axis will provide a sort of selection
rule for the forbidden polaritons in a symmetric DBR pair confined resonant SMC. This could be helpful for finding the hybridization induced polaritons. Our calculation shows the existence of HH subband dominated polaritons which have the quantum numbers \( n=1, n'=2, j_h=\frac{3}{2}, n_{ex} = 2, l = 1 \) with splitting value \( \sim 0.2 \) mev. The details and other interesting results will be published elsewhere.

V. CONCLUDING REMARKS

In conclusion, we have presented a self-consistent semiclassical approach for exciton-polaritons in a QW embedded in an SMC. In this approach, the effect of the complex valence band structure and the non-locality of the dielectric response of the exciton in the QW are carefully considered. For 1HH excitons and normal incidence, our approach gives the same results as those obtained previously. For complex cases such as high index excitons and oblique incidence we expect that it could predict some new phenomena. For example, we have shown that a 2P exciton can also couple to a photon mode and form a polariton. Moreover our analysis gives a "selection rule" for the formation of exciton-polaritons in a symmetric SMC, which is essentially an interplay among the angular quantum numbers of excitons, the electron-hole subbands indices and the resonance conditions of the SMC.

ACKNOWLEDGMENTS

The authors are grateful to Drs. Jizhong Lou, Shaojin Qin and Bangfen Zhu for beneficial discussions and kind help. The authors acknowledge support from the Chinese Academy of Sciences.
REFERENCES

* Present address: Physics Department, University of Michigan.

1. C. Weisbuch, M. Nishioka, A. Ishikawa, and Y. Arakawa, Phys. Rev. Lett. 69, 3314-3317 (1992)

2. R. Houdre, R. P. Stanley, U. Oesterle, M. Ilegems, and C. Weisbuch, Phys. Rev. B 49, 16761-16764 (1994)

3. T. B. Norris, J.-K. Rhee, C.-Y. Sung, Y. Arakawa, M. Nishioka, and C. Weisbuch, Phys. Rev. B 50, 14663 (1994)

4. V. Savona, Z. Hradil, A. Quattropani, and P. Schwendimann, Phys. Rev. B 49, 8774 (1994)

5. J. Tignon, P. Voisin, C. Delalande, M. Voos, R. Houdre, U. Oesterle, and R. P. Stanley, Phys. Rev. Lett. 74, 3967 (1995)

6. T. B. Norris, J.-K. Rhee, C.-Y. Sung, Y. Arakawa, M. Nishioka, and C. Weisbuch, Phys. Rev. B 50, 14663 (1994)

7. S. Pau, G. Björk, J. Jacobson, H. Cao, and Y. Yamamoto, Phys. Rev. B 51, 7090 (1995)

8. S. Pau, G. Björk, J. Jacobson, H. Cao, and Y. Yamamoto, Phys. Rev. B 51, 14437 (1995)

9. A. Fainstein, B. Jusserand, and V. Thierry-Mieg, Phys. Rev. Lett. 75, 3764 (1995)

10. Y. Chen, A. Tredicucci, and F. Bassani, Phys. Rev. B 52, 1800 (1995)

11. T. A. Fisher, A. M. Afshar, D. M. Whittaker, M. S. Skolnick, J. S. Roberts, G. Hill, and M. A. Pate, Phys. Rev. B 51, 2600 (1995)

12. G. Panzarini and L. C. Andreani, Phys. Rev. B 52, 10780 (1995)

13. F. Tassone, C. Piermarocchi, V. Savona, A. Quattropani, and P. Schwendimann, Phys. Rev. B 53, R7642 (1996)
14 T. A. Fisher, A. M. Afshar, M. S. Skolnick, D. M. Whittaker, and J. S. Roberts Phys. Rev. B 53, R10469 (1996)

15 V. Savona and C. Weisbuch Phys. Rev. B 54, 10835 (1996)

16 M. R. Vladimirova, A. V. Kavokin, and M. A. Kaliteevski Phys. Rev. B 54, 14566 (1996)

17 R. P. Stanley, R. Houdre, C. Weisbuch, U. Oesterle, and M. Ilegems Phys. Rev. B 53, 10995 (1996)

18 Y. Zhu et. al. Phys. Rev. Lett. 64, 2499 (1990)

19 F. Tasson, F. Bassani and L. C. Andreani, Il Nuovo Cimento 12, 1673 (1990)

20 L. J. Sham, 2nd Inter. Conf. on MSS-II (Japan) 573 (1985)

21 J. N. Shulman and Y. C. Chang, Phys. Rev. B 31, 2056 (1985)

22 Bangfeng Zhu and Huang K., Phys. Rev. B 36, 8102 (1988)

23 Bangfeng Zhu, Phys. Rev. B 37, 4687 (1988)

24 L. Andreani and A. Pasquarello, Phys. Rev. B 42, 8828 (1990)

25 L. Viña, R. T. Collins, F. E. Mendez, and W. I. Wang, Phys. Rev. Lett. 58, 832 (1987); R. T. Collins, L. Viña, W. I. Wang, L. L. Chang, L. Esaki, K. v. Klitzing, and K. Ploog, Phys. Rev. B 36, 1531 (1987)

26 Ansheng Liu, Phys. Rev. B 50, 8569 (1994), ibid 55, 7101 (1994)

27 A. Yariv, Optical Waves in Crystal: Propagation and Control of the Laser Radiation, Wiley, New York (1984)

28 O. Keller, Phys. Rev. B 37, 10588 (1988)

29 J. M. Luttinger, W. Kohn, Phys. Rev. 97, 869 (1954)

30 Hui Tang and Kun Huang, Journal of Semiconductors 8, 1 (1987) (in Chinese), see also
E.I Ivchenko and G.E.Pikus, *Superlattices and other Heterostructures*, Springer-Verlag, Berlin (1994)

31 G.D. Mahan, *Many Particle Physics*, 2nd edition, Plenum, New York (1990)

32 Gu Xu, Dingzhou Li, Bingshen Wang and Zhao-bin Su, to be published.
FIGURES

FIG. 1. Schematics of the symmetric planar semiconductor microcavity

FIG. 2. The summed Coulomb interacting electron-hole bubble diagram series

APPENDIX A: THE TRANSFER MATRIX ELEMENTS AND GREEN'S
FUNCTIONS.

The transfer matrix elements can be calculated straightforwardly as

\[
    t_{11}^L = e^{-iq_{\perp,1}L_1} \left[ \cos(q_{\perp,2}L_2) - \frac{i}{2} \left( \frac{\varepsilon_2q_{\perp,1}}{\varepsilon_1q_{\perp,2}} + \frac{\varepsilon_1q_{\perp,2}}{\varepsilon_2q_{\perp,1}} \right) \sin q_{\perp,2}L_2 \right]
\]

\[
    t_{12}^L = e^{iq_{\perp,1}L_1} \left[ -\frac{i}{2} \left( \frac{\varepsilon_2q_{\perp,1}}{\varepsilon_1q_{\perp,2}} - \frac{\varepsilon_1q_{\perp,2}}{\varepsilon_2q_{\perp,1}} \right) \sin q_{\perp,2}L_2 \right]
\]

\[
    t_{21}^L = e^{-iq_{\perp,1}L_1} \left[ \frac{i}{2} \left( \frac{\varepsilon_2q_{\perp,1}}{\varepsilon_1q_{\perp,2}} - \frac{\varepsilon_1q_{\perp,2}}{\varepsilon_2q_{\perp,1}} \right) \sin q_{\perp,2}L_2 \right]
\]

\[
    t_{22}^L = e^{iq_{\perp,1}L_1} \left[ \cos(q_{\perp,2}L_2) - \frac{i}{2} \left( \frac{\varepsilon_2q_{\perp,1}}{\varepsilon_1q_{\perp,2}} + \frac{\varepsilon_1q_{\perp,2}}{\varepsilon_2q_{\perp,1}} \right) \sin q_{\perp,2}L_2 \right]
\]

(A1)

and

\[
    t_{11}^R = t_{11}^L, \quad t_{22}^R = t_{22}^L, \quad t_{12}^R = -t_{21}^L, \quad t_{21}^R = -t_{12}^L.
\]

(A2)

Moreover, the Green’s functions in Eq. (2.13) can also be easily solved as

\[
    G_{x,x}(\omega, q_\parallel; z, z') = -\frac{ie^2}{2\omega \varepsilon_c(\omega) q_\perp e^{iq_{\perp,1}|z-z'|}}
\]

\[
    G_{x,z}(\omega, q_\parallel; z, z') = G_{z,x}(\omega, q_\parallel; z, z') = \frac{ie^2}{2\omega \varepsilon_c(\omega) q_\parallel} \text{Sgn}(z-z') e^{iq_{\perp,1}|z-z'|}
\]

\[
    G_{z,z}(\omega, q_\parallel; z, z') = \frac{e^2}{\omega \varepsilon_c(\omega)} \delta(z-z') - \frac{ie^2}{2\omega \varepsilon_c(\omega) q_\perp} e^{iq_{\perp,1}|z-z'|}
\]

\[
    G_{y,y}(\omega, q_\parallel; z, z') = -\frac{i}{2q_\perp} e^{iq_{\perp,1}|z-z'|}
\]

\[
    G_{xy} = G_{yx} = G_{yz} = G_{zy} = 0
\]

(A3)
APPENDIX B: OUTLINE OF THE DERIVATION OF THE POLARIZATION PROPOAGATOR

We outline here the main steps for deriving Eq. (3.4) by a summation over the Coulomb interaction ladder diagrams accommodated in a bubble diagram consisting of a conduction electron and a valence hole, as shown in Fig. 2.

We introduce the second quantized wave operator and current operator:

\[
\hat{\psi}(\vec{r}) = \sum_b \sum_\lambda \sum_s \sum_\alpha \phi_{b,\lambda}^{(h,\lambda)}(\vec{r}) u_\alpha^{(b)}(\vec{r}) c_{s,\alpha}^{(h,\lambda)} \\
\hat{j}(\vec{r}) = \frac{e\hbar}{2imc} (\hat{\psi}^\dagger(\vec{r}) \nabla \hat{\psi}(\vec{r}) - \nabla \hat{\psi}(\vec{r}) \hat{\psi}(\vec{r}))
\]

in which \(\hat{c}_{s,\alpha}^{(h,\lambda)}\) is the second quantized electron annihilation operator for a state with band index \(c, \lambda\) and quantum number \(s\). Note that we dropped the index \(k\) of the cell-periodic functions of the Bloch function, in corresponding with the envelope function approximation.

Using the linear response theory approximation and the Masterabara representation, the polarization part of the electron system \(\pi_r(\omega; \vec{r}, \vec{r}')\) can be expressed as

\[
\pi_r(\omega; \vec{r}, \vec{r}') = -\int_0^\infty d\tau e^{i\omega_n \tau} Tr \{ \hat{\rho} \hat{j}(\vec{r}, \tau) \hat{j}(\vec{r}', 0) \} \big|_{i\omega_n \to \omega + i\eta}
\]

where \(\hat{\rho}\) is the thermal density matrix, \(Tr\) the trace operation, and \(T_r\) the chronological operation along the imaginary time axis. Expression (B3) has the advantage that it can be calculated systematically by applying the diagrammatical technique. We notice first that each pair of electron and hole lines in the upper series of diagrams in Fig. 2 contributes a term

\[
1 - n(\xi_s^{(c,\lambda)}) - n(\xi_{s'}^{(v,\lambda')}) \\
\frac{i\omega_n - \xi_s^{(c,\lambda)}}{-\xi_s^{(c,\lambda)} - \xi_{s'}^{(v,\lambda')}}
\]

where \(s'\) describes the quantum numbers charge conjugated to \(s\). Each pair of electron and hole lines in the lower series of diagrams in Fig. 3 with the directions of the arrows reversed, contributes a term

\[
-1 - n(\xi_s^{(c,\lambda)}) - n(\xi_{s'}^{(v,\lambda')}) \\
\frac{i\omega_n + \xi_s^{(c,\lambda)}}{\xi_s^{(c,\lambda)} + \xi_{s'}^{(v,\lambda')}}
\]

in which \(\xi_s^{(c,\lambda)} = \varepsilon_s^{(c,\lambda)} + E_g - \mu, \xi_s^{(v,\lambda)} = \varepsilon_s^{(v,\lambda)} + \mu\) and \(n(\xi)\) is the Fermi distribution function for the conduction electrons and valence holes. Moreover, a dotted Coulomb line contributes
a factor
\[ u^{\lambda,\lambda'; \lambda''; \lambda'''}_{\alpha, \alpha'} = \sum_{\alpha, \alpha'} \int d^3r d^3r' \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(c, \lambda')}_{s', \alpha'}(\vec{r}) \frac{1}{\varepsilon_c |\vec{r} - \vec{r}'|} \varphi^{(v, \lambda)}_{s', \alpha'}(\vec{r}) \varphi^{(v, \lambda''; \lambda''')}_{s''; \alpha''}(\vec{r}') \] (B6)
where \( \varepsilon_c = \varepsilon_c(\omega) \) is the background dielectric constant for the medium. Finally, each vertex at the end point of the bubble contributes a dipole matrix element \( \langle c, \alpha|\vec{p}|v, \alpha' \rangle \) or \( \langle v, \alpha'|\vec{p}|c, \alpha \rangle \). All the above expressions follow straightforwardly from the quantum many-body text-book with an additional consideration shown in \([B3]\), i.e. our basis wave function is not the usual simple plane wave, but the envelope function associated with a more ”microscopic” cell periodic function \( u \).

It should also be noticed that, for an intrinsic semiconductor in the low excitation limit, the conduction band is almost completely empty and the valence band almost completely full, so the two Fermi distribution functions in Eqs. \([B4]\) and \([B5]\) can be taken as zero. Furthermore, this guarantees that only the ladder diagrams give any contribution\[1]. Through summation over the Coulomb interacting ladder diagrams accommodated in a bubble diagram which consist of a conduction electron and a valence hole (shown in Fig. 2), we can obtain the following expression for the polarization tensor, after a direct but lengthy calculation,
\[ \frac{\pi}{\varepsilon_m^2} \sum_{\alpha, \alpha'} \sum_{\lambda, \lambda'} \sum_{\lambda', \lambda''; \lambda'''} \left\{ \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(v, \lambda')}_{s', \alpha'}(\vec{r}) \langle v, \alpha'|\vec{p}|c, \alpha \rangle \right. \\
- \left. \frac{1}{i\omega_n - \xi^{(c, \lambda)}_{s, \alpha} - \xi^{(v, \lambda')}_{s', \alpha'}} \Gamma^{\lambda, \lambda'}_{s, s'}(i\omega_n; \vec{r}') \right\}, \] (B7)
\[ \Gamma^{\lambda, \lambda'}_{s, s'}(i\omega_n; \vec{r}') = \sum_{\alpha''; \alpha'''} \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(v, \lambda')}_{s', \alpha'}(\vec{r}) \langle c, \alpha''|\vec{p}'|v, \alpha''' \rangle + (-e^2) \sum_{\lambda''; \lambda'''} \sum_{\lambda'''; \lambda''''} u^{\lambda'', \lambda'''}_{s, s''} \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \langle v, \alpha''|\vec{p}'|c, \alpha''' \rangle, \] (B8)
\[ \tilde{\Gamma}^{\lambda, \lambda'}_{s, s'}(i\omega_n; \vec{r}') = \sum_{\alpha''; \alpha'''} \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(v, \lambda')}_{s', \alpha'}(\vec{r}) \langle v, \alpha''|\vec{p}'|c, \alpha''' \rangle - (-e^2) \sum_{\lambda''; \lambda'''} \sum_{\lambda'''; \lambda''''} u^{\lambda'', \lambda'''}_{s, s''} \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \varphi^{(c, \lambda)}_{s, \alpha}(\vec{r}) \langle v, \alpha''|\vec{p}'|c, \alpha''' \rangle \]
can now be derived as
\[ \psi_{\gamma';\gamma} = \frac{1}{i\omega_n + \xi'_{\gamma';\gamma}} \frac{1}{i\omega_n + \xi'_{\gamma,\gamma'}E_{\gamma'}(\omega_n)} \Gamma_{\gamma';\gamma}(\omega_n; \vec{r}', \vec{r}) . \] (B9)

We then introduce two auxiliary functions
\[ P_{\alpha',\alpha}(i\omega_n; \vec{r}, \vec{r}'; \vec{r}'') = \sum_{\lambda,\delta} \sum_{\lambda',\delta'} \varphi^{(c,\lambda)}_{\lambda',\lambda} (\vec{r}') \varphi^{(s,\lambda')}_{\lambda',\delta'} (\vec{r}') \] \[ \frac{1}{i\omega_n - \xi'_{\lambda,\lambda'} - \xi'_s} \Gamma_{\lambda',\lambda}^{(s,\lambda')}(\omega_n; \vec{r}, \vec{r}') \] (B10)
and
\[ \tilde{P}_{\alpha',\alpha}(i\omega_n; \vec{r}, \vec{r}'; \vec{r}'') = \sum_{\lambda,\delta} \sum_{\lambda',\delta'} \varphi^{(c,\lambda)}_{\lambda,\lambda} (\vec{r}) \varphi^{(s,\lambda')}_{\lambda',\delta'} (\vec{r}) \] \[ \frac{1}{i\omega_n + \xi'_{\lambda,\lambda'} + \xi'_s} \Gamma_{\lambda',\lambda}^{(s,\lambda')}(\omega_n; \vec{r}, \vec{r}') . \] (B11)

We can express \( \Gamma^{(s,\lambda)}_{\lambda',\lambda}(i\omega_n, \vec{r}'') \) and \( \tilde{\Gamma}^{(s,\lambda)}_{\lambda',\lambda}(i\omega_n, \vec{r}'') \) in terms of the two auxiliary functions by utilizing the orthogonal properties of \( \varphi^{(c,\lambda)}_{\lambda,\lambda} (\vec{r}) \) and \( \varphi^{(s,\lambda')}_{\lambda',\delta'} (\vec{r}) \), in a way similar to an inverse generalized Fourier transformation in the Hilbert space. We have further the completeness relation for \( \varphi^{(c,\lambda)}_{\lambda,\lambda} (\vec{r}) \) and \( \varphi^{(s,\lambda')}_{\lambda',\delta'} (\vec{r}) \). With the aid of these procedures, the polarization tensor can now be derived as
\[ \tilde{\Pi}(\omega_n; \vec{r}, \vec{r}'') = \left( \frac{m}{\hbar} \right)^2 \sum_{\alpha,\alpha'} \left\{ \langle v, \alpha | \tilde{p} | c, \alpha \rangle P_{\alpha,\alpha'}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') - \langle c, \alpha | \tilde{p} | v, \alpha' \rangle \tilde{P}_{\alpha,\alpha'}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') \right\} . \] (B12)

Next, we apply the operator \( i\omega_n \delta_{\alpha,\alpha'^{m}} \delta_{\alpha',\alpha'^{m}} - [H_0]_{\alpha,\alpha'^{m} ; \alpha,\alpha'^{m}} \) to the \( P_{\alpha',\alpha'^{m}}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') \) from the left, apply the operator \( i\omega_n \delta_{\alpha'^{m} ; \alpha} \delta_{\alpha'^{m} ; \alpha} + [H_0]_{\alpha'^{m} ; \alpha,\alpha} \) to \( \tilde{P}_{\alpha',\alpha'^{m}}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') \) from the right, and obtain
\[ \left\{ \langle v, \alpha' | \tilde{p} | c, \alpha \rangle \delta(\vec{r} - \vec{r}'') \delta(\vec{r}' - \vec{r}'') \right\} \] \[ P_{\alpha',\alpha'^{m}}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') = \langle c, \alpha | \tilde{p} | v, \alpha' \rangle \delta(\vec{r} - \vec{r}'') \delta(\vec{r}' - \vec{r}'') \] \[ \sum_{\alpha'^{m}} \sum_{\alpha'^{m}} \tilde{P}_{\alpha',\alpha'^{m}}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') \left\{ \langle v, \alpha' | \tilde{p} | c, \alpha \rangle \delta(\vec{r} - \vec{r}'') \delta(\vec{r}' - \vec{r}'') \right\} \] \[ \tilde{P}_{\alpha,\alpha'^{m}}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') = \langle c, \alpha | \tilde{p} | v, \alpha' \rangle \delta(\vec{r} - \vec{r}'') \delta(\vec{r}' - \vec{r}'') . \] (B13)

We may then solve the auxiliary functions from Eqs. \( (B13) \) and \( (B13) \) by the Green’s function method to get
\[ P_{\alpha,\alpha'}(i\omega_n; \vec{r}, \vec{r}; \vec{r}'') = \sum_{\beta,\beta'} G_{\alpha,\alpha' ; \beta,\beta'}(i\omega_n; \vec{r}, \vec{r}; \vec{r}; \vec{r}'') \langle c, \beta | \tilde{p} | v, \beta' \rangle \] (B14)
with
\[ G_{\alpha,\alpha'^{m}; \beta,\beta'}(i\omega_n; \vec{r}, \vec{r}; \vec{r}; \vec{r}'') = \sum_{\lambda, \lambda'} \sum_{s, s'} \sum_{n} \psi^{(s,\lambda';\lambda',\alpha'^{m})}_{\alpha,\alpha'^{m}}(\vec{r}, \vec{r}) \psi^{(s,\lambda';\lambda',\alpha'^{m})}_{\beta,\beta'}(\vec{r}, \vec{r}') \] \[ \frac{1}{i\omega_n - E_{n}^{(\lambda, \lambda'; s, s')}} \] (B15)
as well as

\[ \tilde{P}_{\alpha,\alpha'}(i\omega_m; \vec{r}, \vec{r}'; \vec{r}'') = \sum_{\beta,\beta'} \langle \nu, \beta'| \bar{p} c, \beta \rangle \tilde{G}_{\beta,\beta';\alpha,\alpha'}(i\omega_m; \vec{r}', \vec{r}; \vec{r}) \]  \hspace{1cm} (B16)

with

\[ \tilde{G}_{\beta,\beta';\alpha'';\alpha'}(i\omega_m; \vec{r}, \vec{r}'; \vec{r}, \vec{r}'') = \sum_{\lambda,s} \sum_{\lambda',s'} \psi^{(\lambda,s;\lambda',s';n)}(\vec{r}, \vec{r}'') \psi^{*(\lambda,s;\lambda',s';n)}(\vec{r}, \vec{r}') \frac{i\omega_m + E^{(\lambda,s;\lambda',s')}}{i\omega_m} \]  \hspace{1cm} (B17)

in which \( \psi^{(\lambda,s;\lambda',s';n)}(\vec{r}, \vec{r}'') \) and \( E^{(\lambda,s;\lambda',s')} \) are exactly those introduced in Eq.(3.8). By substituting Eqs. (B14)-(B17) into Eq.(B12), we obtain Eq.(3.6) as desired.
Fig. 1 of Xu et al., "Semiclassical..."
Fig. 2 of Xu et al., "Semiclassical..."

\[
\begin{align*}
\text{c:e} & \quad \text{conduction electron} \\
\text{v:h} & \quad \text{valence hole} \\
\text{Coulomb interaction} & \\
\end{align*}
\]