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#### Communication

# To the theory of hybrid organics/semiconductor nanostructures in microcavity



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#### ABSTRACT

We consider the hybrid structure in microcavity where the energy of Frenkel exciton in organic layer is equal to the energy of Wannier – Mott exciton in semiconductor quantum well (QW). The exciton located in QW of semiconductor layer can interact with molecules of organic layer and under influence of this interaction can change the position jumping and exciting one of organic molecules. The exciton located in molecule of organic layer also can change the position jumping to semiconductor QW. The number of such jumps depends on the intensity of interaction. In the paper we consider the influence of direct coulomb dipole-dipole interaction and indirect interaction through the optical field of microcavity on the kinetics of excitation. It was shown that the dispersion of hybrid states are modified by coulomb interaction particularly when the distance between layers is enough small. The lowest branch of dispersion curves with deep minimum at nonzero wave vector may be useful in the studies of the condensation of low energy hybrid excitations.

#### 1. Introduction

The investigation of polariton states in resonant hybrid nanostructures containing organic and inorganic molecules is important because the new hybrid states can be tailored to engineer the fluorescence efficiency and relaxation processes in many applications. In such hybrid nanostructures the distance between organic and inorganic parts of hybrid nanostructure can be small and, for example, Frenkel exciton from organic layer can transport his energy to empty place in semiconductor QW creating Wannier exciton and such process can take place also in opposite direction when Wannier exciton creates the Frenkel exciton in one of organic molecules. Actually such processes are similar to numerous jumps of molecular excitation in organic crystal. However, the life time of Frenkel exciton in organic part of hybrid structure and the life time of Wannier exciton in semiconductor part can be different because for both are different their interaction with the nearest layer. Optical pumping of one of component of hybrid structure can stimulate high intensity of non radiate energy transfer between the components of hybrid structure and can be important for creation of strong light-emitting efficiency. The organic/inorganic hybrid structures are described in many published papers. However, in the majority of these publications (see for instance [1-11]) the considered hybrid structures have the excitation energy of Frenkel exciton much lower than the excitation energy of Wannier exciton. For this reason after high energy pumping of semiconductor layer and fast

Wannier exciton energy relaxation the excitation energy is concentrated in the layer with Frenkel exciton and its emission. The different situation was considered in published papers [12,13]. In the paper [13] the hybridization and energy transformation were considered when organic and inorganic layers are in microcavity and when the level of energy of 2D Frenkel exciton and the level of energy of 2D Wannier exciton are near the level of energy of the cavity optical mode. It was shown that interaction through cavity photons creates mixed hybrid Frenkel-Wannier-Mott-cavity photon mode excitations. The pumping of these states by external source was investigated in [14] ( see also the paper [15]). The hybrid organic/semiconductor structure in the limit of strong coupling between Frenkel and Wannier - Mott excitons have been investigated in [16] and it was shown that hybrid structure can have a very large optical nonlinearity. These states may have unusual properties such as large oscillator strength typical for Frenkel excitons and also can have large exciton radii typical for Wannier-Mott excitons.

In this paper we take into account the results obtained in papers [12,13]. We consider the states of Frenkel-Wannier-Mott hybrid nanostructure in microcavity taking into account not only interaction of excitations with the cavity optical mode but also the direct dipole-dipole resonance interaction in hybrid nanostructure important at small distance between organic and semiconductor component. We also show how can be changed the structure of exciton states in hybrid nanostructure when the distance between organic and inorganic layers increases.

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In the next Section 2 the quantum mechanical consideration of the processes in the hybrid organic/semiconductor nanostructure will be developed taking into account the direct coulomb dipole-dipole interaction between exciton and empty place and also the interaction of hybrid structure with cavity optical mode. As the next step in the Sections 3 and 4 we consider the influence of microcavity on the dispersion of hybrid states.

Considering properties of exciton in organic/inorganic hybrid structure it is important to have in mind that distance of mentioned above exciton energy levels to the lowest energy of conductivity zone can be very different for organic and semiconductor components. In the case of organic material this distance can be order of half eV and probability to transfer the energy of exciton to the conductivity zone is negligible. In semiconductor material we have different picture because this distance can be in ten times smaller in comparison with the similar distance for organic material. Nevertheless, as it follows from experiments (see, for instance mentioned papers [1-11]) in many hybrid structures the transfer energy from excited semiconductor thin layer to organic layer even at room temperature can be very fast and efficient. The organic material also can have the large efficiency of transfer energy to semiconductor if the energy of exciton in organic material will be close to the value of energy of exciton in semiconductor material. Thus we can expect that hybrid structure with organic/ inorganic materials which we consider in this paper can have a unique properties and the life time enough large to be considered for the creation of a new devices (see also [14]).

## 2. Resonant organic/semiconductor nanostructure in microcavity

The dispersion equation for hybrid states in cavity with inorganic and organic layers is demonstrated in quantum mechanical approach that was also used in [13]. The Hamiltonian for the hybrid structure in considered case is

$$\begin{split} \hat{H} &= \sum_{k} \left[ \hbar \omega_{W,k} \hat{B}_{W,k}^{+} \hat{B}_{W,k} + \hbar \omega_{F,k} \hat{B}_{F,k}^{+} \hat{B}_{F,k} + \hbar \Omega(k) \hat{B}_{C,k}^{+} \hat{B}_{C,k} + + \right. \\ & \left. \hbar (\Gamma_{W} \hat{B}_{C,k}^{+} \hat{B}_{W,k} + \Gamma_{W}^{*} \hat{B}_{W,k}^{+} \hat{B}_{C,k}) + \hbar (\Gamma_{F} \hat{B}_{C,k}^{+} \hat{B}_{F,k} + \Gamma_{F}^{*} \hat{B}_{F,k}^{+} \hat{B}_{C,k}) \right. \\ & \left. + + \hbar (\Gamma \hat{B}_{W,k}^{+} \hat{B}_{F,k} + \Gamma^{*} \hat{B}_{F,k}^{+} \hat{B}_{W,k}) \right] \end{split}$$

$$(1)$$

Here  $\omega_{W,k}, \omega_{F,k}$ ,  $\Omega(k)$  are frequencies of Wannier-Mott exciton (WME), Frenkel exciton (FRE) and cavity optical mode with the same wave vector k. The functions  $\Gamma_W = \Gamma_W(s,k)$ ,  $\Gamma_F = \Gamma_F(s,k)$  are dependent on k and s – half of distance between IQW and OQW. Here we have introduced an additional term with function  $\Gamma = \Gamma(s,k)$  for coulomb interaction. Such function was absent in [13]. The dependences  $\Gamma_W = \Gamma_W(s,k)$ ,  $\Gamma_F = \Gamma_F(s,k)$ ,  $\Gamma(s,k)$  will be defined in Sections 3, 4. To diagonal Hamiltonian (1) we introduce the new operators  $\hat{\xi}_{\sigma}(k)$ ,  $\hat{\xi}_{\sigma}^{\dagger}(k)$  by using the canonical transformation with norm equation

$$\begin{split} \hat{B}_W(k) &= \sum_{\sigma} \varPhi_{\sigma,W}(k) \hat{\xi}_{\sigma}(k), \\ \hat{B}_F(k) &= \sum_{\sigma} \Phi_{\sigma,F}(k) \hat{\xi}_{\sigma}(k) \hat{B}_c(k) = \sum_{\sigma} \Phi_{\sigma,C}(k) \hat{\xi}_{\sigma,C}(k), \\ \sum_{\sigma} \left[ |\Phi_{\sigma,W}|^2 + |\Phi_{\sigma,F}|^2 + |\Phi_{\sigma,C}|^2 \right] = 1, \end{split} \tag{2}$$

The functions  $\Phi_{\sigma,w}$ ,  $\Phi_{\sigma,F}$ ,  $\Phi_{\sigma,C}$  are defined as solutions of set of correspondent linear equations with frequencies  $\omega$  of new hybrid states that are defined from equation of equality to zero of determinant of this set

$$\begin{split} (\omega_W - \omega) \Phi_W + & \Gamma \Phi_F + \Gamma_W \Phi_C = 0, \\ & \Gamma^* \Phi_W + (\omega_F - \omega) \Phi_F + \Gamma_F \Phi_C = 0, \\ & \Gamma_W^* \Phi_W + \Gamma_F^* \Phi_F + (\Omega - \omega) \Phi_C = 0, \end{split} \tag{3a}$$

$$\begin{vmatrix} \frac{\omega_{W} - \omega}{\Gamma_{W}^{*}, & \frac{\Gamma}{\Gamma_{F}^{*}}, & \frac{\Gamma}{\Gamma_{F}^{*}}, & \frac{\Gamma}{\Gamma_{W}^{*}} \end{vmatrix} = 0$$
(3b)

The terms with  $\Gamma$  were absent in [13]. Eq. (3b) of third order in frequency may be written now in the following form

$$\begin{split} & [\Omega(k) - \omega] [(\omega_{W} - \omega)(\omega_{F} - \omega) - |\Gamma|^{2}] - \\ & - |\Gamma_{W}|^{2} (\omega_{F} - \omega) - |\Gamma_{F}|^{2} (\omega_{W} - \omega) + \Theta = 0 \\ & \Theta = \Gamma \Gamma_{W} \Gamma_{F} + \Gamma^{*} \Gamma_{W}^{*} \Gamma_{F}^{*}. \end{split} \tag{4}$$

The second factor in first term (4) may be transformed to new frequencies

$$\omega^2 - \omega(\omega_W + \omega_F) - \omega_W \omega_F - |\Gamma|^2 = (\omega - \nu_W)(\omega - \nu_F), \tag{5a}$$

$$\nu_{W}(s, k) = \frac{\omega_{W} + \omega_{F}}{2} + \sqrt{(\frac{\omega_{W} - \omega_{F}}{2})^{2} + |\Gamma(s, k)|^{2}},$$
(5b)

$$\nu_{\rm F}(s,k) = \frac{\omega_{\rm W} + \omega_{\rm F}}{2} - \sqrt{(\frac{\omega_{\rm W} - \omega_{\rm F}}{2})^2 + |\Gamma(s,k)|^2} \,. \tag{5c}$$

The dependence on distance and wave vector is the following. Then Eq. (4) has the following form

$$[\Omega(k) - \omega)[(\nu_{W} - \omega)(\nu_{F} - \omega)] - \tag{6}$$

$$-|\Gamma_{W}|^{2}(\omega_{F}-\omega)-|\Gamma_{F}|^{2}(\omega_{W}-\omega)+\Theta=0$$

Dividing (6) on factor  $(\nu_W-\omega)(\nu_F-\omega)$  leads dispersion equation to the following form

$$[\Omega(k) - \omega] - \frac{|\Gamma_{\mathbf{W}}|^2 (\omega_{\mathbf{F}} - \omega) + |\Gamma_{\mathbf{F}}|^2 (\omega_{\mathbf{W}} - \omega) - \Theta}{(\nu_{\mathbf{W}} - \omega)(\nu_{\mathbf{F}} - \omega)} = 0$$
(7)

with new resonances at frequencies (5b) and (5c). This equation easily can be transformed to more simple equation (see [17]). The result is the following:

$$\left[\Omega(k) - \omega\right] + \frac{\left|\widetilde{\Gamma}_{W}(s, k)\right|^{2}}{\omega - \nu_{W}(s, k)} + \frac{\left|\widetilde{\Gamma}_{F}(s, k)\right|^{2}}{\omega - \nu_{F}(s, k)} = 0,$$
(8a)

$$\left|\widetilde{\Gamma}_{W}(s, k)\right|^{2} = \frac{\left|\Gamma_{W}\right|^{2}(\omega_{F} - \nu_{W}) + \left|\Gamma_{F}\right|^{2}[\omega_{W} - \nu_{W}] - \Theta}{(\nu_{F} - \nu_{W})},\tag{8b}$$

$$\widetilde{|\Gamma_{F}(s, k)|^{2}} = \frac{|\Gamma_{W}|^{2}(\omega_{F} - \nu_{F}) + |\Gamma_{F}|^{2}[\omega_{W} - \nu_{F}] - \Theta}{(\nu_{W} - \nu_{F})}.$$
(8c)

Now we can consider the limiting case of exact resonance when the frequencies  $\omega_W$  and  $\omega_F$  in microcavity are equal, i.e.  $\omega_W = \omega_F = \omega_0$ . In this case Eq. (5b, c) are transformed to the following relations.  $\nu_W(s, k) = \omega_0 + |\Gamma(s, k)|, \ \nu_F(s, k) = \omega_0 - |\Gamma(s, k)|,$ 

and as the result the equations Eq. (8b) and Eq. (8c) are transformed to the following relations

$$\left|\widetilde{\Gamma}_{\mathrm{W}}(s,\,k\right|^{2} = \frac{\left[\left|\Gamma_{\mathrm{W}}\right|^{2} + \left|\Gamma_{\mathrm{F}}\right|^{2}\right]\left[-\left|\Gamma(s,\,k)\right|\right] - \left[\Gamma(s,\,k)\Gamma_{\mathrm{W}}^{*}\Gamma_{\mathrm{F}} + \Gamma^{*}(s,\,k)\Gamma_{\mathrm{W}}\Gamma_{\mathrm{F}}^{*}\right]}{\left(-2\left|\Gamma(s,\,k)\right|\right)}.$$

$$\widetilde{\left|\Gamma_{\mathrm{F}}(s,\,k\right|^{2} = \frac{[|\Gamma_{\mathrm{W}}|^{2} + |\Gamma_{\mathrm{F}}|^{2}][|\Gamma(s,\,k)|] - [\Gamma(s,\,k)\Gamma_{\mathrm{W}}^{*}\Gamma_{\mathrm{F}} + \Gamma^{*}(s,\,k)\Gamma_{\mathrm{W}}\Gamma_{\mathrm{F}}^{*}]}{(2|\Gamma(s,\,k)|)}$$

or to the equations

$$\left|\widetilde{\Gamma}_{\mathrm{W}}(s,k)\right|^{2} = \frac{1}{2} \left[ |\Gamma_{\mathrm{W}}|^{2} + |\Gamma_{\mathrm{F}}|^{2} + \frac{\Gamma(s,k)\Gamma_{\mathrm{W}}^{*}\Gamma_{\mathrm{F}} + \Gamma^{*}(s,k)\Gamma_{\mathrm{W}}\Gamma_{\mathrm{F}}^{*}}{|\Gamma(s,k)|} \right],$$

$$\left|\widetilde{\Gamma}_{\rm F}(s,\,k)\right|^2 = \frac{1}{2} \left[ |\Gamma_{\rm W}|^2 + |\Gamma_{\rm F}|^2 - \frac{\Gamma(s,\,k) \Gamma_{\rm W}^* \Gamma_{\rm F} + \Gamma^*(s,\,k) \Gamma_{\rm W} \Gamma_{\rm F}^*}{|\Gamma(s,\,k)|} \right]$$

The last terms defines energy of coulomb interaction. However, as it is seen from these equations the intensity  $\left|\widetilde{\Gamma}_{W,F}(s,k)\right|^2$  in numerators of fractions in Eq. (11) are not dependent on s and k due to reduction of modules  $|\Gamma(s,k)|$  including s and k in numerators and denominators of fractions. The main role of direct coulomb interaction is concentrated

in frequencies  $\nu_W(s,\,k),\,\nu_F(s,\,k)$  that define denominators in Eq. (8a). In the same time it is seen some redistribution of intensity between  $|\widetilde{\Gamma}_W|^2$  and  $|\widetilde{\Gamma}_F|^2$  in comparison with distribution  $|\Gamma_W|^2$  and  $|\Gamma_F|^2$ . For real positive  $\Gamma,\,\Gamma_W,\Gamma_F$  these values correspond to the following relations.

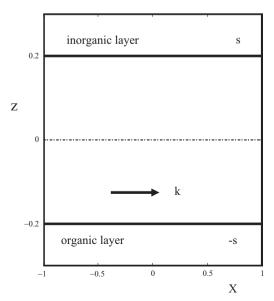
 $(\widetilde{\Gamma}_{\mathrm{W}})^2 = \frac{1}{2} [\Gamma_{\mathrm{W}} + \Gamma_{\mathrm{F}}]^2, \ (\widetilde{\Gamma}_{\mathrm{F}})^2 = \frac{1}{2} [\Gamma_{\mathrm{W}} - \Gamma_{\mathrm{F}}]^2.$ 

Now it is interesting to consider in more details the peculiarities of the unusual properties of hybrid resonant structures with the same energy of excitons of two different layers. Considering such structure we can assume that the energy of Frenkel exciton in organic layer and the energy of Wannier - Mott exciton in semiconductor layer are the same and the influence of coulomb interaction can be strong. The exciton located in one of layer under influence of this interaction can change the position jumping to another layer and as we have mentioned the number of such jumps depends on the intensity of coulomb interaction. It is interesting to understand what type of dispersion curve can be created in the pumping of such resonant hybrid structure. As the energies of exciton will  $\nu_{\rm W}(s, k) = \omega_0 + |\Gamma(s, k)|$  or  $\nu_{\rm F}(s, k) = \omega_0 - |\Gamma(s, k)|$  we can expect that the splitting in dispersion curve will be small in comparison with the value of main frequency. However, the splitting can be large in comparison with width of pumping signal. In this case interaction of pumping light with one of excited state in microcavity can be strong. If the splitting is small the interaction of light with excitation can be less interesting. The interaction between layers with participation of excitons can have an interest particularly in structures where the distance between organic and semiconductor thin layers is enough small and when the splitting of energy of exciton is large. The study for the dispersion of excitons in considered case can be useful. We present below only simplest picture of mentioned dispersion curves (see Section 4).

#### 3. Coulomb interaction in hybrid structure

In the paper [13] the coulomb interaction was considered when the borders are absent. In this section we shall investigate the influence of microcavity only on the coulomb interaction. The influence of interaction of hybrid structure with cavity optical photons will be considered later. In the beginning now it is convenient to consider the case when microcavity is absent.

The investigated structure is shown on Fig. 1. It is formed by inorganic and organic thin layers divided by distance  $z_0 = 2s > 0$ . The arrow shows the wave vector k and polarization of electric field in x



 $\textbf{Fig. 1.} \ \ \textbf{Organic/inorganic} \ \ \textbf{structure} \ \ \textbf{where} \ \ \textbf{Frenkel} \ \ \textbf{exciton} \ \ \textbf{or} \ \textbf{Wannier-Mott} \ \ \textbf{exciton} \ \ \textbf{may} \ \ \textbf{be} \ \ \textbf{generated}.$ 

direction. The total Hamilton operator  $\hat{H}$  in wave vector k space may be written as

$$\hat{\mathbf{H}} = \sum_{k} \left[ E_{W,k}(k) B_{W,k}^{+} \mathbf{B}_{W,k} + E_{F,k} B_{F,k}^{+} \mathbf{B}_{F,k} + (\langle F, k | \hat{\mathbf{H}}_{int} | W, k \rangle B_{F,k}^{+} \mathbf{B}_{W,k} + h.c. \right]$$
(9)

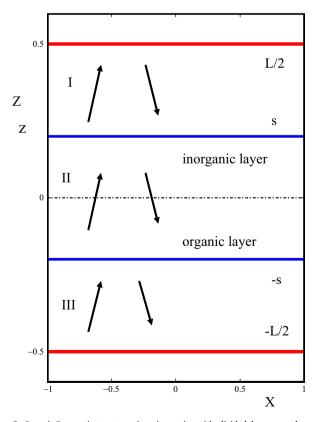
The first and second terms in (9) include energy of excitation  $E_{W,k}$  for WM exciton and  $E_{F,k}$  for FR exciton with operators of exciton creation (annihilation)  $B_{W,k}^+(B_{W,k})$ ,  $B_{F,k}^+(B_{F,k})$ . The last term in (9) defines energy of coulomb interaction. The solutions of the Schrodinger equation  $\hat{H}\psi = E\psi$  with energy E was presented in [12] for L – modes with polarization along wave vector and as final result can be used the following expression for matrix element  $\langle F, k|\hat{H}_{int}|W, k\rangle$  in (9) with extremely small width of semiconductor. In this case the matrix element in (9) has the following form

$$\langle F, k | \hat{\mathbf{H}}_{\text{int}} | W, k \rangle = \hbar \Gamma(k) = \operatorname{S} \operatorname{kexp}(-k \mathbf{z}_0),$$
 (10)

$$S = \frac{P_F^{(0)} P_W^{(0)}}{a_F a_W},\tag{11}$$

Where  $P_{F,W}^{(0)}$  are matrix elements of dipole transition in organic and semiconductor, and  $a_{F,W}$  are the cell constant of organic and WM exciton radii. It must be noted that factor S in right side of the expression (10) is multiplication on two parts one of which is defined only by IQW parameters and the second only by organic layer parameters. The dependence Eq. (10) on wave vector includes the increasing k and the decreasing  $\exp(-kz_0)$ . As the result the product of these factors has maximum  $\exp(-1)/z_0$  at  $k=k_{\rm max}=1/z_0$ . This maximum shifts in region of high wave vectors and increases as  $1/z_0$  when the distance between IQW and organic layer is decreasing.

We will use in our consideration the microcavity with both totally reflecting sides in z region L/2 > z > -L/2 that is shown on Fig. 2. Two layers are in symmetrical positions in relation to center of cavity at z=0.



**Fig. 2.** Organic/inorganic structure in microcavity with divided by space planes of organic and inorganic materials where Frenkel exciton or Wannier-Mott exciton may be generated.

Generation of WM exciton is possible in upper IQW demonstrated by line at co-ordinate z = s. Generation of FR exciton is possible in lower organic layer demonstrated by line at co-ordinate z = -s. The electric fields E(x) of hybrid states have common space x dependence  $E(x) = E(0)\exp(ikx)$  with common wave vector k.

We assume that the borders of microcavity are totally reflecting the field like mirror and that in the cavity the field of dipoles on mirror sides is equal zero. For one border and semi-infinite media one dipole "creates" the second "image of dipole" that is symmetrical in relation to mirror. For two borders the same dipole can "create" the infinite series of these "images of dipoles". Calculation of  $\Gamma(s, k)$  with taking into account full set of these "images dipoles" gives following form of  $\Gamma(s, k)$ 

$$\Gamma(s,\,k) = \frac{1}{\hbar} [\frac{P_W^{(0)} P_F^{(0)}}{a_W a_F} k [e^{-2ks} + \sum_{n=1}^{} (-1)^n [e^{-kR_n^{(1)}} + e^{-kR_n^{(2)}}]]], \eqno(12)$$

where

$$R_n^{(1)} = nL - (s)[1 + (-1)^n], \ R_n^{(2)} = nL + (s)[1 + (-1)^n].$$
 (13)

Substitution (13) to (12) and summation of geometrical progression of exponents gives the following form of  $\Gamma(s, k)$ 

$$\Gamma(s,k) = \frac{1}{\hbar} \frac{P_{W}^{(0)} P_{F}^{(0)}}{a_{W} a_{F}} k \left[ e^{-kz_{0}} - 2e^{-kL} \frac{1}{1 - e^{-2kL}} + (e^{-2ks} + e^{2ks}) \frac{e^{-2kL}}{1 - e^{-2kL}} \right]. \tag{14}$$

The transformation (14) gives the following function  $\Gamma(k)$ 

$$\Gamma(s, k) = \Gamma_{Dir} L\Psi(k), \tag{15}$$

where

$$\Gamma_{\text{Dir}} = \frac{1}{\hbar} \frac{P_{\text{W}}^{(0)} P_{\text{F}}^{(0)}}{\text{awarL}}, \ \Psi(k) = k \left\{ 2 \frac{\left\{ \text{sh} \left[ \frac{k}{2} (L - 2\text{s}) \right] \right\}^{2}}{\text{sh(kL)}} \right\},$$

We consider below the expression (15) for  $\Gamma(s, k)$  in some limiting cases. In the case, when distance 2s=L, i.e. when layers are placed near cavity borders where field is equal zero the value  $\Gamma(L/2, k) = 0$ . In the limiting case of extremely large L the main functions that determine the value  $\Gamma(s, k)$  are increasing exponents, depending on L,

$$\Gamma(s, k) = \frac{1}{\hbar} \frac{P_W^{(0)} P_F^{(0)}}{a_W a_F} k \left[ 2 \frac{\left[ \left( \frac{1}{2} \right) \exp\left[ \frac{k}{2} (L - 2s) \right] \right]^2}{\left( \frac{1}{2} \right) \exp(kL)} \right]. \tag{16}$$

It is easy to see that the function  $\Gamma(s,k)$  at large L exactly coincides with (11) after exponents reduction in (16).

$$\Gamma(s, k) = \frac{1}{\hbar} \frac{P_W^{(0)} P_F^{(0)}}{a_W a_F} \Psi_0(k), \ \Psi_0(k) = k \exp(-ks)$$

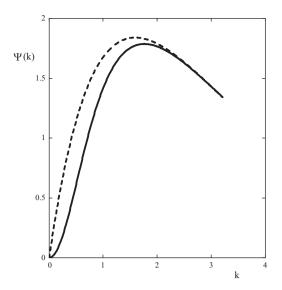
It is of interest dependence of the function  $\Gamma(s, k)$  on the wave vector for small k and definite s. In this case

$$\Gamma(s,k) = \frac{1}{\hbar} \frac{P_W^{(0)} P_F^{(0)}}{a_W a_F} k \frac{k}{2} (\frac{(L-2s)^2}{L}). \tag{17}$$

It is seen from (17) that in this case energy of direct interaction is proportional to square of wave vector, that is distinguish from [12] where this function is linear. Analyses of (15) show, that in this case, the same as in [12], at increasing k function  $\Gamma(s,k)$  is increasing and then after maximum exponentially goes down. The functions  $\Psi_0(k)$  and  $\Psi(k)$  in the non dimensional units  $kL/\pi$  are shown on Fig. 3 for s/L=0.1 as dashed and solid curves. It is seen that in the cavity in comparison with free space the energy of direct coulomb interaction is decreasing and its maximum is shifted in region of large wave vectors.

#### 4. Dispersion of the resonance hybrid states

The direct instantaneous coulomb interaction was investigated in the previous Section 3 without taking into account retarded interaction between layers through photons of microcavity. The all above presented calculations gave the possibility to obtain in this final section the dispersion of the hybrid states in microcavity taking into account the borders of microcavity and also the coulomb and photon interaction



**Fig. 3.** The dependence  $\Psi(k)$  that determines the energy of direct coulomb interaction between exciton and empty layer. The sold line indicates  $\Psi(k)$  for layers in microcavity. The dashed line indicates  $\Psi(k)$  without cavity. It is seen that microcavity decreases the value  $\Psi(k)$  and shifts its maximum to region of larger wave vectors.

between different nanostructures in microcavity. Following calculation procedure used in [13] we shall investigate polariton states in microcavity with organic/semiconductor structure that contain in development of [13] layers divided by finite space between layers, varying up to cavity width, with accordingly varying coulomb interaction between them. The scheme of microcavity with organic/semiconductor structure is shown on Fig. 2. The electrical fields of longitudinal L-mode can be considered in the regions I (L/2 > z > s), II (s > z > -s) and III (-s > z > -L/2) of Fig. 2 as sums of two waves with opposite in sign z components of wave vectors

$$E_{I} = A_{I}e^{i\beta z} + A_{2}e^{-i\beta z}, \ E_{II} = A_{3}e^{i\beta z} + A_{4}e^{-i\beta z}, \ E_{III} = A_{5}e^{i\beta z} + A_{6}e^{-i\beta z}, \eqno(18)$$

where function  $\beta = \sqrt{(\omega/c)^2 - k^2}$ .

The equations of equality to zero for field on the "mirror" borders  $z = \pm L/2$  give relations between amplitudes A<sub>1</sub>, A<sub>2</sub> and A<sub>5</sub>,A<sub>6</sub>

$$A_2 = -\mu A_1, A_5 = -\mu A_6, \mu = e^{i\beta L}.$$
 (19)

The equation of continuity for amplitudes of electric fields on the border between regions I and II gives equation that determines relation between amplitudes  $A_{1,2,3,4}$ 

$$A_1 e^{i\beta s} + A_2 e^{-i\beta s} = A_3 e^{i\beta s} + A_4 e^{-i\beta s},$$
(20)

The equation of continuity for amplitudes of electric fields on border between regions II and III gives equation that determine the relation between amplitudes  $A_{3,4,5,6}$ 

$$A_3 e^{-i\beta s} + A_4 e^{i\beta s} = A_5 e^{-i\beta s} + A_6 e^{i\beta s}, \tag{21}$$

Next relations between the same amplitudes can be obtained from equations of continuity for y component of magnetic field  $H_y=(ic/\omega)(\partial E_x/\partial z).$  These equations include polarization  $P_W(\omega,\,k)$  of IQW and  $P_F(\omega,\,k)$  of OQW

$$[A_1 e^{i\beta s} - A_2 e^{-i\beta s}] - [A_3 e^{i\beta s} - A_4 e^{-i\beta s}] = -\left(\frac{4\pi}{i\beta}\right) \left(\frac{\omega}{c}\right)^2 P_W(\omega, k). \tag{22a}$$

$$[A_3 e^{-i\beta s} - A_4 e^{i\beta s}] - [A_5 e^{-i\beta s} - A_6 e^{i\beta s}] = -\left(\frac{4\pi}{i\beta}\right) \left(\frac{\omega}{c}\right)^2 P_F(\omega, k). \tag{22b}$$

The polarization  $P_F(\omega, k)$  is determined by field  $A_1e^{i\beta s} + A_2e^{-i\beta s}$  and the polarization  $P_F(\omega, k)$  is determined by field  $A_5e^{-i\beta s} + A_6e^{i\beta s}$ 

$$P_{W}(\omega, k) = \chi_{W}(\omega, k)[A_{1}e^{i\beta s} + A_{2}e^{-i\beta s}], \qquad (23a)$$

$$P_{F}(\omega, k) = \chi_{F}(\omega, k) [A_5 e^{-i\beta s} + A_6 e^{i\beta s}]. \tag{23b}$$

Polarization abilities  $\chi_{W,F}(\omega,k)$  have the following forms with oscillator strength  $f_{W,F}$  that are connected with  $\Gamma_{W,F}$ 

$$\begin{split} \chi_{\mathrm{W}}(\omega,\,k) &= \frac{\mathrm{f}_{\mathrm{W}}}{\nu_{\mathrm{W}}(k) - \omega}, \ |\Gamma_{\mathrm{W}}|^2 = \frac{4\pi\Omega}{L} \mathrm{f}_{\mathrm{W}} \\ \chi_{\mathrm{F}}(\omega,\,k) &= \frac{\mathrm{f}_{\mathrm{F}}}{\nu_{\mathrm{F}}(k) - \omega}, \ |\Gamma_{\mathrm{F}}|^2 = \frac{4\pi\Omega}{L} \mathrm{f}_{\mathrm{F}}. \end{split} \tag{24}$$

where  $\nu_{\rm W}(k)$ ,  $\nu_{\rm F}(k)$  are frequency of coulomb excitons (see Section 2). The system of all equations can be transformed to the only two equations for  $A_3A_4$ .

Two equations that define relations between  $A_{1,2,3,4}$  and  $A_{3,4,5,6}$ , have the following forms

$$[A_{1}e^{i\beta s} - A_{2}e^{-i\beta s}] - [A_{3}e^{i\beta s} - A_{4}e^{-i\beta s}] = -\left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2} \chi_{W}(\omega, k)[A_{1}e^{i\beta s} + A_{2}e^{-i\beta s}]$$
(25a)

$$[A_{3}e^{-i\beta s} - A_{4}e^{i\beta s}] - [A_{5}e^{-i\beta s} - A_{6}e^{i\beta s}] = -\left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2} \chi_{F}(\omega, k)[A_{5}e^{-i\beta s} + A_{6}e^{i\beta s}]$$
(25b)

Using relation (19) between amplitudes  $A_1$  and  $A_2$ , we obtain system of two Eq. (20) and (25a) in the following forms

$$A_1(e^{i\beta s} - \mu e^{-i\beta s}) = A_3 e^{i\beta s} + A_4 e^{-i\beta s},$$
(26a)

$$A_{1}[e^{i\beta s} + \mu e^{-i\beta s}] - [A_{3}e^{i\beta s} - A_{4}e^{-i\beta s}] = -\left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2} \chi_{F}(\omega, k) A_{1}[e^{i\beta s} - \mu e^{-i\beta s}].$$
(26b)

In the same time using relation (19) between amplitudes  $A_5$  and  $A_6$ , we obtain system of two Eqs. (21) and (25b) in the following forms

$$A_6(-\mu e^{-i\beta s} + e^{i\beta s}) = A_3 e^{-i\beta s} + A_4 e^{i\beta s}, \tag{27a}$$

$$A_{6}[e^{i\beta s} + \mu e^{-i\beta s}] + [A_{3}e^{-i\beta s} - A_{4}e^{i\beta s}] = -\left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2} \chi_{F}(\omega) A_{6}[e^{i\beta s} - \mu e^{-i\beta s}].$$
(27b)

Substitution  $A_1$  from (26a) as function  $A_3$   $\mu$   $A_4$  to Eq. (26b) gives first equation connecting only  $A_3$   $\mu$   $A_4$ . Substitution  $A_6$  from (27a) as function  $A_3$  and  $A_4$  to Eq. (27b) gives second equation connecting only the same  $A_3$   $\mu$   $A_4$ . These two equations have following forms

$$\begin{split} A_{3}[2\mu + \left(\frac{4\pi}{i\beta}\right) & \left(\frac{\omega}{c}\right)^{2} \chi_{W}(\omega, k) (e^{2i\beta s} - \mu)] + A_{4}[2\\ & + \left(\frac{4\pi}{i\beta}\right) & \left(\frac{\omega}{c}\right)^{2} \chi_{W}(\omega, k) (1 - \mu e^{-2i\beta s})] = 0 \end{split} \tag{28a}$$

$$A_{3}\left[2 + \left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2}\chi_{F}(\omega)(1 - \mu e^{-2i\beta s})\right] + A_{4}\left[2\mu + \left(\frac{4\pi}{i\beta}\right)\left(\frac{\omega}{c}\right)^{2}\chi_{F}(\omega)(e^{2i\beta s} - \mu)\right]$$

$$= 0 \tag{28b}$$

Using these two equations we can find their determinant and corresponding equation which can be used for the investigation of properties of hybrid structure. Dispersion equation of hybrid excitations in considered case is

$$(\mu^{2}-1) = -\frac{1}{2} \left(\frac{4\pi}{i\beta}\right) \left(\frac{\omega}{c}\right)^{2} (\chi_{W} + \chi_{F}) [-\mu^{2} + 2\mu \cos(2\beta s) - 1] - \frac{1}{4} \left[\frac{4\pi}{i\beta} \left(\frac{\omega}{c}\right)^{2}\right]^{2} \chi_{W} \chi_{F} [(e^{2i\beta s} - \mu)^{2} - (1 - \mu e^{-2i\beta s})^{2}].$$
(29)

Left part of (29) is equal zero at  $\mu=-1$ , i.e. at  $\beta L=\pi$ . The product  $\chi_W \chi_F$  is equal to the sum of the same two resonances of  $\chi_W$  and  $\chi_F$  with some coefficients

$$\chi_{\mathbf{W}}(\omega, k)\chi_{\mathbf{F}}(\omega, k) = \left(\frac{[L/(4\pi\Omega)]|\Gamma_{\mathbf{W}}|^2}{\nu_{\mathbf{W}}(k) - \nu_{\mathbf{F}}(k)}\right)\chi_{\mathbf{F}}(\omega, k) + \left(\frac{[L/(4\pi\Omega)]|\Gamma_{\mathbf{F}}|^2}{\nu_{\mathbf{F}}(k) - \nu_{\mathbf{W}}(k)}\right)\chi_{\mathbf{W}}(\omega, k).$$
(30)

The frequency of optical mode of microcavity is a zero of left side of Eq. (29) and it is defined by equation  $\beta L = \pi$ . We shall use expansion on small deviation of  $\beta L$  from this critical value, i.e. we assume, that  $\beta L = \pi + \delta$  with small deviation from resonance  $\delta$ . Due to equation  $\mu = e^{i(\pi+\delta)} = -(1+i\delta)$  the factor in left side of (29) which is going to zero has the form  $\mu + 1 = -i\delta$ . Then the left side of (29) at  $\mu - 1 = -2$  near zero has the form  $\mu^2 - 1 = 2i\delta$  with  $\delta = \beta L - \pi$ . The right part of (29) may be considered at  $\mu = -1$  and as result for the dispersion Eq. (29) we obtain

$$2i(\beta L - \pi) = -\frac{1}{2} \left( \frac{4\pi}{i\beta} \right) (\frac{\omega}{c})^2 (\chi_W + \chi_F) [-2 - 2\cos(2\beta s)] - \frac{1}{4} \left[ \frac{4\pi}{i\beta} (\frac{\omega}{c})^2 \right]^2 \chi_W \chi_F [(e^{2i\beta s} + 1)^2 - (1 + e^{-2i\beta s})^2],$$
(31)

01

$$\beta L - \pi = -\left(\frac{4\pi}{\beta}\right) \left(\frac{\omega}{c}\right)^2 (\chi_1 + \chi_2) [\cos(\beta s)]^2 + \left[\left(\frac{4\pi}{\beta}\right) \left(\frac{\omega}{c}\right)^2\right]^2 \chi_W$$

$$\chi_F \sin(2\beta s) [\cos(\beta s)]^2. \tag{32}$$

Now we have to take into account that the left side of Eq. (29) is equal zero at frequency  $\omega = \Omega + \varepsilon$ ,  $\Omega > \varepsilon$  where  $\Omega(k) = c\sqrt{(\pi/L)^2 + k^2}$  is frequency of cavity optical mode and hence  $\beta L - \pi = (L/c)[\omega - \Omega(k)]$ . After such reconstruction the dispersion Eq. (29) has the following form

$$\omega - \Omega(k) = -\left(\frac{4\pi\Omega}{L}\right) (\chi_{W} + \chi_{F}) [\cos(\beta s)]^{2}$$

$$+ \left[\frac{(4\pi\Omega)^{2}}{Lc}\right] \chi_{W} \chi_{F} \sin(2\beta s) [\cos(\beta s)]^{2}.$$
(33)

Using the relation (30) it is simple to separate resonances  $\chi_W$  and  $\chi_F$ . In this case we obtain the final formula for dispersion equation

$$\begin{split} \omega - \Omega(k) &= \{ -(\frac{4\pi\Omega}{L}) + [\frac{(4\pi\Omega)^2}{Lc}] [\frac{[L/(4\pi\Omega)] ||F||^2}{\nu_F(k) - \nu_W(k)}] \sin(2\pi s/L) \} [\cos(\pi s/L)]^2 \chi_W \\ &\qquad (\omega, k) + \\ &+ \{ -(\frac{4\pi\Omega}{L}) + [\frac{(4\pi\Omega)^2}{Lc}] [\frac{[L/(4\pi\Omega)] ||FW||^2}{\nu_W(k) - \nu_F(k)}] \sin(2\pi s/L) \} [\cos(\pi s/L)]^2 \chi_F(\omega, k). \end{split}$$

$$(34)$$

In limiting case of s=0 when  $\Gamma(k)$  is equal zero and IQW and organic layer are in the cavity center dispersion Eq. (34) has the same form that was found in [13]

$$\omega - \Omega(k) = \left(\frac{\Gamma_{W}^{2}}{\omega - \omega_{W}}\right) + \left(\frac{\Gamma_{F}^{2}}{\omega - \omega_{F}}\right), \,. \tag{35}$$

Eq. (34) is cubic equation with relation to frequency  $\omega$ . It is seen that introduced in Section 2 functions  $\Gamma_{W,F}(s,k)$  are defined by following equations

$$|\Gamma_{W}(s, k)|^{2} = \left\{ -\left(\frac{4\pi\Omega(0)}{L}\right) + \left[\frac{(4\pi\Omega(0))^{2}}{Lc}\right] - \left[\frac{f_{F}}{\nu_{F}(k) - \nu_{W}(k)}\right] \sin(2\pi s/L) \right\} \left[\cos(\pi s/L)\right]^{2} f_{W},$$
(36a)

$$\begin{split} |\Gamma_{\rm F}(s,k)|^2 &= \{-\left(\frac{4\pi\Omega(0)}{\rm L}\right) + \left[\frac{(4\pi\Omega(0))^2}{\rm Lc}\right] \\ &= \left[\frac{\rm f_W}{\nu_{\rm W}(k) - \nu_{\rm F}(k)}\right] \sin(2\pi s/L) \} \left[\cos(\pi s/L)\right]^2 \rm f_{\rm F}. \end{split} \tag{36b}$$

Then the Eq. (34) has the following form

$$\omega - \Omega(k) = \left(\frac{|\Gamma_{W}(s, k)|^{2}}{\nu_{W}(s, k) - \omega}\right) + \left(\frac{|\Gamma_{F}(s, k)|^{2}}{\nu_{F}(s, k) - \omega}\right). \tag{37}$$

In the case of strong resonance when  $\nu_W(s, k) = \omega_0 + |\Gamma(s, k)|$  and

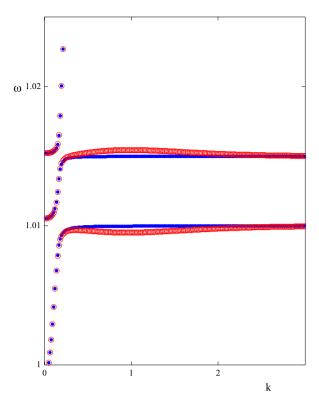


Fig. 4. Dispersion curves of hybrid excitations are shown for half of distance s/L=0.4 between inorganic and organic layers. The curves presented by thick blue points correspond to hybrid branches at zero energy of direct interaction. The curves presented by big red circles correspond to hybrid branches at non zero direct interaction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

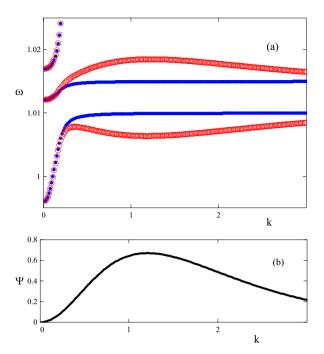
 $\nu_{\rm F}(s, k) = \omega_0 - |\Gamma(s, k)|$  the Eq. (34) has the following form

$$\omega - \Omega(k) = \left(\frac{|\Gamma_{W}(s, k)|^{2}}{\omega_{0} + |\Gamma(s, k)| - \omega}\right) + \left(\frac{|\Gamma_{F}(s, k)|^{2}}{\omega_{0} - |\Gamma(s, k)| - \omega}\right). \tag{38}$$

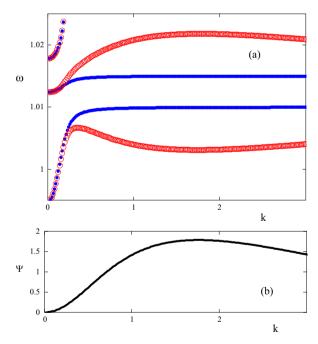
Solution of this cubic in frequency Eq. (38) was performed by standard procedure. The non dimensional variables  $\widetilde{\omega}=\omega/\Omega(0),\,\widetilde{k}=kL/\pi$  were used like [13]. We have used also the parameters of the same order that were used in [13]  $\Gamma_F=12~\text{meV}/\hbar,\,\,\Gamma_W=8.4~\text{meV}/\hbar,\,\,\Omega(0)=1.5~\text{eV}/\hbar,\,\pi/L=2.4\text{cm}^{-1}$  with  $\omega_W/\Omega(0)=1.015,\,\omega_F/\Omega(0)=1.01,$ 

 $\Gamma_F/\Omega(0)=8\times 10^{-3}, \Gamma_W/\Omega(0)=5.6\times 10^{-3}.$  It is seen multiplicative peculiarity of frequency factor  $\Gamma_{\rm Dir}$  in (15) in relation to WM and FR parameters  $P_{W,F}^{(0)}/a_{W,F}$  with the same position of parameter L for  $\Gamma_{\rm Dir}$  in (19) as  $\Gamma_{W,F}$  in (24). Therefore non dimensional parameter of direct interaction is equal  $\Gamma_{\rm Dir}/\Omega(0)=\sqrt{\Gamma_W\Gamma_F}/\Omega(0)=6.7\times 10^{-3}.$ 

The dispersion curves of hybrid excitations are shown at Figs. 4–7. The Figs. 3-7 are shown with introduced non dimensional units. The set of blue thick points on Figs. 4-7 show dispersion dependences that were found without coulomb interaction. The set of light red rings demonstrate dispersion dependences that were calculated with taking into account coulomb interaction. The Fig. 4 demonstrates results at s/L = 0.4, when the IQW and organic layer are near cavity borders with zero field and polariton splitting is extremely small. It is seen beginning of arising small pit and hump in lowest and middle in frequency branches. The pit was shown first in [13]. The dispersion curves with pit and hump with extreme values at non zero wave vector are seen more distinctly on the Fig. 5a for decreasing s/L = 0.2. Fig. 5b demonstrates dependence  $\Psi(k)$  for the same distance s/L = 0.2. It is seen that wave vector of maximum  $\Psi(k)$  is coincide with wave vector of pit and hump on Fig. 5a. Fig. 6a for s/L = 0.1 demonstrates that pit and hump in comparison with Fig. 5 are increasing and are shifting to region of increasing wave vectors in agreement with dependences

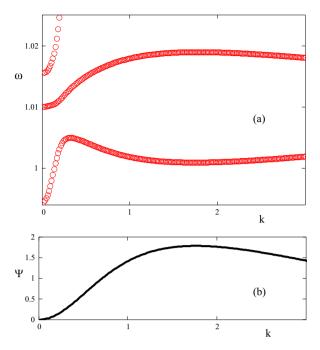


**Fig. 5.** Dispersion curves of hybrid excitations are shown on Fig. 5a for half distance s/L = 0.2 between layers. The dependence  $\Psi(k)$  for the same s/L = 0.2 is shown on Fig. 5b. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



**Fig. 6.** Dispersion curves of hybrid excitations are shown on Fig.6a for half distance s/L = 0.1 between organic and inorganic layers. The dependence  $\Psi(k)$  for the same s/L = 0.1 is shown on Fig.6b. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

 $k_{max}=1/s$ ,  $\Gamma_{max}\approx 1/s$ . The dependence  $\Psi(k)$  for this distance s/L=0.1 is shown on Fig. 6b. Comparison of Figs. 4–6 demonstrates that appearance of pit and hump in dispersion curves is caused by coulomb interaction between IQW and organic layer. Dispersion dependence with pit may be interesting for investigation of Bose condensation effect for hybrid excitations. It is seen that in region of small wave vectors low frequency hybrid branch before pit has linear dependence from wave vector. Fig. 7a,b demonstrate dispersion curves at s/L=0.1 for strong resonance with exactly equal frequencies  $\omega_W/\Omega(0)=\omega_F/\Omega(0)=1.01$ .



**Fig. 7.** The dispersion curves for s/L=0.1 at strong resonance with equal frequencies  $\omega_W/\Omega(0) = \omega_F/\Omega(0) = 1.01$  for non zero direct interaction are shown on Fig. 7a and corresponding dependence  $\Psi(k)$  is shown on Fig. 7b. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 7b demonstrates dependence  $\Psi(k)$  with maximum at wave vector of pit and hump on Fig. 7a.

#### 5. Conclusion

We investigated optical hybrid polaritonic states in microcavity with organic/semiconductor nanostructures and obtained the results that may be useful for devices tailoring. It was considered nanostructures with finite distance between organic layer and semiconductor layer in which can be generated resonating of Frenkel exciton,

Wannier-Mott exciton and photon of optical cavity mode. The value of distance between organic layer and semiconductor layer defines intensity of direct coulomb interaction between layers and electric field of optical mode for cavity with "mirror" borders. Decreasing of distance leads to drastically increasing of direct coulomb interaction and determine increasing of electric field in optical mode. It was shown that one dispersion branch has deep minimum at non zero wave vector, that may be interesting for condensation of such hybrid states.

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