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Kosterlitz – Thouless phase transition in microcavity polariton system

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Kosterlitz – Thouless phase transition in the system of exciton-polaritons in microcavity is studied. Transition temperature to superfluid state was found as function of exciton-photon detuning. Non quadratic dispersion law was taken into account in the framework of self-consistent harmonic approximation (SCHA).

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System of exciton-polaritons in optical microcavity became actual last time both from fundamental and applied points of view.

The system under study is an optical microcavity in which the semiconductor quantum well is embedded. Quasi-two-dimensional excitons in the quantum well can be resonantly excited by photons of optical microcavity. As a result at large Q-factor of optical microcavity composite particles, exciton-polaritons, superposition of microcavity photons and excitons are formed in the system (see [1] and references therein). At low density exciton-polaritons with the large accuracy can be treated as bosons, and in this quasi-2D system with decreasing of temperature Kosterlitz – Thouless [2 – 4] topological transition should occur into superfluid state with quasi-long range phase order. Interesting property of this system is that exciton-polariton in the microcavity can posses very small effective mass, defined by, depending on geometry of an optical microcavity, dispersion law at small longitudal momentum (see below). Therefore the transition temperature, inversely proportional to the effective mass can reach room temperatures. But after transition of polariton system in a phase with quasi-long range order the photons leaving optical microcavity should possess statistics of laser radiation. In this sense the specified system, considered as a source of radiation, is the laser without inversion of population [6 – 8].

In the system because of its two-dimensionality true Bose-condensation is absent [5] and the transition to the superfluid state as it was already mentioned, is Kosterlitz – Thouless transition. Theory of Kosterlitz – Thouless phase transition developed for systems of particles with quadratic dispersion law. It uses as a first step constructing of "hydrodynamic functional", efficiently describing the system at large scales (where it is essentially renormalized by topological excitations – vortices in locally superfluid liquid). But at construction of this functional it is required to calculate local superfluid density in the framework of *microscopic theory*. Algorithms of its microscopic calculation use quadratic dispersion law of initial (quasi)particles through Landau algorithm of calculating normal component. Note, that only for quadratic dispersion law of particles momentum of normal component, which is calculated in Landau algorithm, is proportional to density of normal component. However for experimentally realizable systems the essential region in which it is possible to consider a polariton spectrum as quadratic, is small, and consequently it is necessary to take into account *non quadratic* spectrum of polaritons.

To overcome this difficulty, we shall describe polariton system by *effective* Hamiltonian with quadratic dispersion law with effective mass depending on temperature. We shall calculate dependence of this mass on temperature using generalization of self-consisted harmonic approximation.

Further, using Kosterlitz – Thouless theory and the theory of the dilute two-dimensional bose gas, we shall calculate dependence of temperature of superfluid phase transition from parameters of a problem (exciton-photon detuning etc.).

1. Self-consistent harmonic approximation for effective mass. The spectrum of exciton-polariton is determined by interaction of two branches: 1) photon in microcavity with dispersion law $\omega(k_{||}) = c\sqrt{k_{||}^2 + (2\pi n/L)^2}$; at small $k_{||}$ we have $\mathcal{E}(k) = E_0 + k_{||}^2/2m_{ph}$, where $E_0 = 2\pi nc/L$,

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$m_{ph} = 2\pi n/cL$; 2) exciton in quantum well with dispersion law $\mathcal{E}(k) = E_g - E_{\text{ex}} + k^2/2m_{\text{ex}}$, E_g is semiconductor gap, E_{ex} is exciton binding energy. Low polariton spectrum is presented on Fig.1. For simplicity

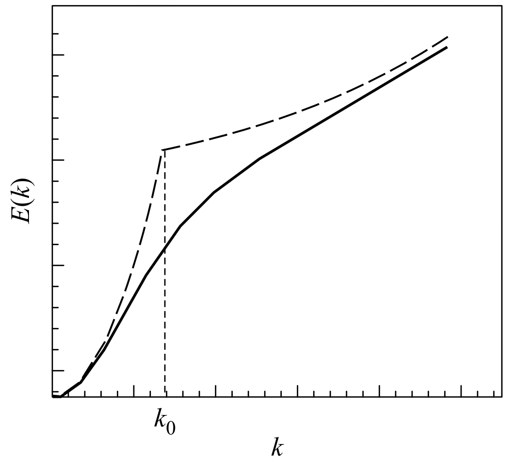

Fig.1 Non-interacting low polariton spectrum

we approximate this spectrum by two parabolas, as can be seen on Fig.1:

$$\begin{aligned} \mathcal{E}(k) &= \frac{k^2}{2m_{\text{eff}}}, \qquad k < k_0; \\ \mathcal{E}(k) &= E + \frac{k^2}{2m_{\text{ex}}}, \quad k > k_0. \end{aligned} \tag{1}$$

where m_{ph} and m_{ex} are photon and exciton mass; here

$$\frac{1}{m_{\text{eff}}} = \frac{m_{\text{ex}} + m_{ph}}{2m_{ph}m_{\text{ex}}} + \frac{(m_{\text{ex}} - m_{ph})E_{dt}}{2m_{ph}m_{\text{ex}}\sqrt{E_{dt}^2 + 4\Omega_p^2}}, \tag{2}$$

$$E = \frac{1}{2}E_{dt} + \frac{1}{2}\sqrt{E_{dt}^2 + 4\Omega_p^2}, \tag{3}$$

$$E_{dt} = E_g - E_{\text{ex}} - E_0, \tag{4}$$

$$k_0 = \sqrt{\frac{2m_{\text{ex}}m_{\text{eff}}E}{m_{\text{ex}} - m_{\text{eff}}}}, \tag{5}$$

where Ω_p – polariton splitting.

As an effective Hamiltonian we shall use Hamiltonian with quadratic dispersion law $\mathcal{E}(k) = \alpha k^2$ and trial parameter α. Effective polariton mass is connected with trial parameter as $\alpha = 1/2m_{\text{pol}}$. Trial parameter α is found by minimization of free energy:

$$F_{\text{trial}} = T \ln \operatorname{Sp} e^{-\widehat{H}_0(\alpha)/T} + \\ + \frac{\operatorname{Sp}(\widehat{H}_0(\alpha) - \widehat{H})e^{-\widehat{H}_0(\alpha)/T}}{\operatorname{Sp} e^{-\widehat{H}_0(\alpha)/T}} = \min. \tag{6}$$

This corresponds to the variant of self-consistent harmonic approximation (SCHA). Here $\widehat{H} = \widehat{T} + \widehat{V}$ is initial Hamiltonian of polariton system, $\widehat{T}$ is energy operator of noninteracting polaritons with nonquadratic dispersion law, $\widehat{V}$ is polariton-polariton interaction. Trial Hamiltonian is choosen in the form of $\widehat{H}(\alpha) = \widehat{T}_0(\alpha) + \widehat{V}$, where $\widehat{T}_0(\alpha)$ is the kinetic energy operator with quadratic dispersion law $\mathcal{E}(k) = \alpha k^2$, the operator of interaction $\widehat{V}$ is not changed[3)]. All calculations is made at fixed temperature and density.

2. Interacting polaritons in two dimensions. At experimentally realizable conditions the polariton system is usually rather rarefied, therefore at calculations we shall use Popov approach which is the generalization of Bogolyubov theory on 2D weakly-interacting Bose-gas. To apply Popov approach to two-dimensional system it is necessary to cut off all integrals in the momenta space at low momentum k_c and after calculations to remove the infrared divergence. In this approach momentum distribution of particles and the spectrum of elementary excitations are given by the following formulae:

$$n(k) = \frac{\varepsilon(k) + \mu - E_b(k)}{2E_b(k)} + \frac{\varepsilon(k) + \mu}{E_b(k)} n_{\text{bose}}(E_b(k)), \tag{7}$$

$$E_b(k) = \sqrt{\varepsilon^2(k) + 2\mu\varepsilon(k)}. \tag{8}$$

Here $\varepsilon(k)$ is the quadratic spectrum αk^2 in effective Hamiltonian (see sec.1) The integral on region $\sim k_c$ at calculation of averages is proportional to k_c^2. Since Popov theory suggest, that $k_c^2 \ll m\mu$, and we are interesting in temperatures much greater than μ, it is possible to replace the low limit of integration with a zero.

Momentum distribution of particles can be separated into two terms. The first term represents depletion of the condensate at zero temperature due to interactions. At calculation of averages it is possible to notice, that there is a ultra-violet divergence. This divergence leads to necessity of renormalization of coupling constant and replacement it by T-matrix, which is describes collision of two particles in vacuum. However we neglect the contribution, corresponding to $T = 0$ since we are interested in high temperatures, where this contribution is small on parameter $\mu/T \ll 1$. The last statement can be easily obtained using expression for the energy density at zero temperature [4]:

$$\mathcal{E} = 4\pi\alpha n^2 / \ln \frac{1}{nr_0^2}. \tag{9}$$

[3)] One can show that T-matrix for polariton-polariton interaction essentially depend on microcavity parameters only at $\Omega_p \ll \ll E_{dt}$, that defines applicability of our theory(more general case will be considered in another paper).

Differentiating eq. (9) over α gives:

$$\langle k^2\rangle_{T=0} \sim \mu^2 \ln\frac{\alpha}{\mu r_0^2}, \tag{10}$$

while temperature average is (see later):

$$\langle k^2\rangle_T \sim T^2. \tag{11}$$

From this estimations we conclude that zero temperature contribution is small. The second term in distribution function (7) gives finite temperature contribution to condensate depletion. Further we shall calculate averages only with this term in distribution function.

The average of k^2 has the following form in SCHA:

$$\langle\hat{k}^2\rangle = 2\pi\int_0^\infty k^2\frac{\varepsilon(k)+\mu}{E_b(k)}n_{\rm bose}(E_b(k))\frac{kdk}{(2\pi)^2} = = \frac{\pi T^2}{(2\pi\hbar^2)^2\alpha^2}\int_0^\infty\frac{\sqrt{x^2+\gamma^2}-\gamma}{e^x-1}dx,\quad \gamma=\frac{\mu}{T}. \tag{12}$$

The average of $\hat{T}$ is given by the following equation:

$$\langle\hat{T}\rangle = \frac{\pi T^2}{2m_{\rm eff}\alpha^2(2\pi\hbar^2)^2}\int_0^\infty\frac{\sqrt{x^2+\gamma^2}-\gamma}{e^x-1}dx - -\frac{\pi T^2 b}{\alpha^2(2\pi\hbar^2)^2}\int_{\epsilon_0}^\infty\frac{\sqrt{x^2+\gamma^2}-\gamma-(E\alpha/bT)}{e^x-1}dx, \tag{13}$$

$$\epsilon_0=\sqrt{(\alpha E/bT)^2+2\gamma(\alpha E/bT)},\quad b=\frac{m_{\rm ex}-m_{\rm eff}}{2m_{\rm ex}m_{\rm eff}}.$$

Let us introduce the following notations for integrals:

$$\mathcal{I}_1(\gamma,\epsilon)=\int_\epsilon^\infty\frac{\sqrt{x^2+\gamma^2}-\gamma}{e^x-1}dx, \tag{14}$$

$$\mathcal{I}_2(\gamma,\epsilon)=\int_\epsilon^\infty\frac{\sqrt{x^2+\gamma^2}-\gamma}{\sqrt{x^2+\gamma^2}(e^x-1)}dx, \tag{15}$$

and use obvious identity:

$$\partial\mathcal{I}_1/\partial\gamma = -\mathcal{I}_2. \tag{16}$$

Derivatives at fixed density are calculated as follows:

$$(2\pi\hbar^2)^2\frac{\partial}{\partial\alpha}\langle\hat{k}^2\rangle = -\frac{2\pi T^2}{\alpha^3}\mathcal{I}_1(\gamma,0)-\frac{\pi T}{\alpha^2}\mathcal{I}_2(\gamma,0)\frac{\partial\mu}{\partial\alpha}, \tag{17}$$

$$(2\pi\hbar^2)^2\frac{\partial}{\partial\alpha}\langle\hat{T}\rangle = = -\frac{\pi T}{2m_{ph}\alpha^2}\left(\frac{2T}{\alpha}\mathcal{I}_1(\gamma,0)+\frac{\partial\mu}{\partial\alpha}\mathcal{I}_2(\gamma,0)\right) + +\frac{\pi Tb}{\alpha^2}\left(\frac{2T}{\alpha}\mathcal{I}_1(\gamma,\epsilon_0)+\frac{\partial\mu}{\partial\alpha}\mathcal{I}_2(\gamma,\epsilon_0)\right) - -\frac{\pi TE}{\alpha^2}\int_{\epsilon_0}^\infty\frac{dx}{e^x-1}, \tag{18}$$

where the derivative $\partial\mu/\partial\alpha$ is necessary to be calculated from the equation of state:

$$n=\frac{\mu}{8\pi\alpha\hbar^2}\ln\frac{\hbar^2\alpha}{\mu r_0^2}-\frac{T}{4\pi\alpha\hbar^2}\mathcal{I}_2(\gamma,0), \tag{19}$$

$$8\pi\hbar^2 n-\frac{\mu}{\alpha}=\frac{\partial\mu}{\partial\alpha}\left(\ln\frac{\hbar^2\alpha}{\mu r_0^2}-1-2\frac{\partial\mathcal{I}_2}{\partial\gamma}\right). \tag{20}$$

Further we are interesting in sufficiently high temperatures, i.e. $\gamma\ll 1$, since in this area we expect transition from normal to superfluid state. The presented system of the equations is rather cumbersome, however it simplifies in the point, corresponding to Kosterlitz – Thouless phase transition. In case of weakly interacting Bose-gas the temperature at this point practically coincides with quasi-condensation temperature and with accuracy $\mathcal{O}(1/\ln(nr_0^2))$ it can be found from the equation (Kosterlitz – Nelson universal jump):

$$n=\frac{T_c}{4\pi\alpha\hbar^2}\ln\frac{T_c}{\mu_c}+\frac{T_c}{\pi\alpha\hbar^2} = =\frac{\mu_c}{8\pi\alpha\hbar^2}\ln\frac{\hbar^2\alpha}{\mu_c r_0^2}-\frac{T_c}{4\pi\alpha\hbar^2}\ln\frac{T_c}{2\mu_c}. \tag{21}$$

Further we shall take into account only leading order in $\gamma_c=\mu_c/T_c$. Then the equation (20) for derivative in leading order will become

$$\frac{T_c}{2\alpha}\ln\frac{T_c}{\mu_c}=\frac{\partial\mu}{\partial\alpha}\frac{T_c}{\mu_c}\ln\frac{T_c}{\mu_c}. \tag{22}$$

As a result the equation of the self-consistency at the transition point has the form:

$$\left(\alpha-\frac{1}{2m_{ph}}\right)(4T_c\mathcal{I}_1(\gamma_c,0)+\mu_c\mathcal{I}_2(\gamma_c,0)) = =2E\alpha\int_{\epsilon_0}^\infty\frac{dx}{e^x-1}-b(4T_c\mathcal{I}_1(\gamma_c,\epsilon_0)+\mu_c\mathcal{I}_2(\gamma_c,\epsilon_0)). \tag{23}$$

To calculate the transition temperature, it is necessary to solve this equation together with the equation of state (19) and the equation (21) for a transition point. Using value of chemical potential and temperature in the transition point it is possible to obtain dependence of phase transition temperature as function of exciton-photon detuning and polariton splitting:

$$T_c = T_{\text{eff}} - \frac{2E}{\mathcal{C}(\gamma_c, 0)} \ln(1 - e^{-\epsilon_0}) - \\ - (T_{\text{eff}} - T_{\text{ex}}) \frac{\mathcal{C}(\gamma_c, \epsilon_0)}{\mathcal{C}(\gamma_c, 0)}, \quad (24)$$

where $\mathcal{C}$, ϵ_0 and γ_c equals:

$$\mathcal{C}(\gamma, \epsilon) = 4 \int_{\epsilon}^{\infty} \frac{\sqrt{x^2 + \gamma^2} - \gamma}{e^x - 1} + \\ + \gamma \int_{\epsilon}^{\infty} \frac{\sqrt{x^2 + \gamma^2} - \gamma}{\sqrt{x^2 + \gamma^2}(e^x - 1)}, \quad (25)$$

$$\epsilon_0 = \sqrt{\left(\frac{E}{T_{\text{eff}} - T_{\text{ex}}}\right)^2 + 2\gamma_c \left(\frac{E}{T_{\text{eff}} - T_{\text{ex}}}\right)}, \quad (26)$$

$$\gamma_c = \frac{4 \ln \ln(1/nr_0^2)}{\ln(1/nr_0^2)} \quad (27)$$

and T_{eff} and T_{ex} are transition temperatures for systems with masses m_{eff} and m_{ex} respectively:

$$T_c = \frac{2\pi\hbar^2 n}{m \ln \ln(1/nr_0^2)}. \quad (28)$$

When E increases, occupation of “exciton” part of spectrum at given temperature decreases, thus effective mass of polariton decreases. As a result temperature of Kosterlitz – Thouless phase transition for two-dimensional polariton system increases in according with equation (28). The resulting dependence from E is depicted on Fig.2. As we expected, at small E

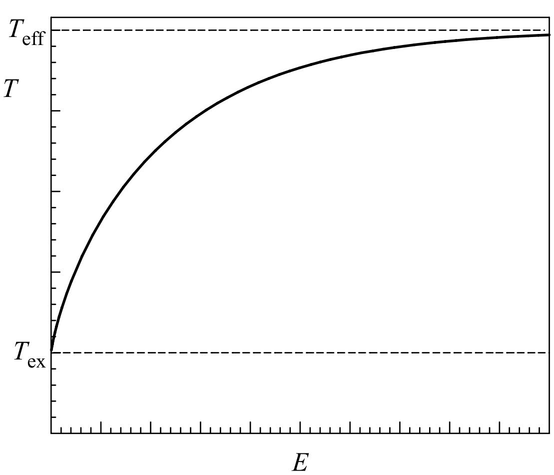

Fig.2 Dependence of the superfluid transition temperature on E

the superfluid transition temperature is close to that in exciton system and it is logarithmically growing when E is increasing. At the large E the transition temperature slightly differs from that in system with mass m_{eff}. Dependence T_c on E_{dt} and Ω_p is presented on Fig.3.

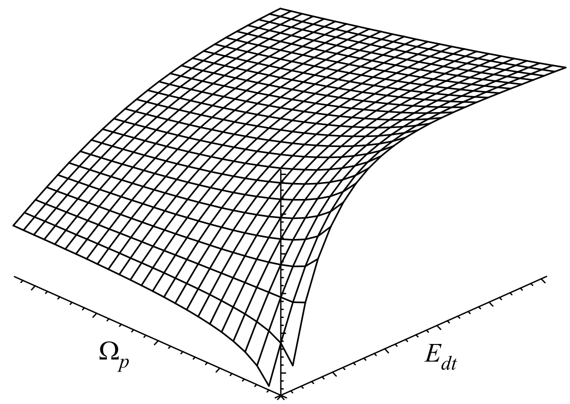

Fig.3 Dependence of the superfluid transition temperature on detuning E_{dt} and polariton splitting Ω_p (see text)

3. Conclusion. The superfluid phase transition in the system of exciton-polariton in optical microcavity with embedded semiconductor quantum well is considered. For determination of the transition temperature we used the variant of self-consistent harmonic approximation and calculated the dependence of effective exciton-polariton mass from exciton-photon detuning in phase transition point. By this approach essential non-quadratic of dispersion law of exciton-polaritons is taken into account.

Note, that now in experiment, by virtue of insufficient value of microcavity Q-factor, quasi-equilibrium state of microcavity polaritons probably is not reached yet. However we expect, that the dependences predicted in the present work will be found experimentally after further improvement of microcavity Q-factor.

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