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LETTER TO THE EDITOR

Bose–Einstein condensation of excitons in a semiconductor quantum well

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Abstract. We consider the problem of Bose–Einstein condensation of excitons in a single quantum well with infinitely high potential barriers. A formal treatment similar to BCS theory of superconductivity is used to calculate the chemical potential of excitons in the Bose-condensed ground state as a function of quantum-well thickness in a low-density limit.

Over the past 30 years the problem of Bose–Einstein condensation of excitons has been the subject of considerable experimental and theoretical interest. In view of the great advances made in our ability to design and manufacture low-dimensional semiconductor structures, the search for a low-dimensional condensed phase of excitons has greatly expanded in recent years. Most of the works have studied the exciton condensed phase in low-dimensional structures in which the electrons and holes are in two different infinitesimally thin layers separated by a wide barrier material (Zhu *et al* 1995, Naveh and Laikhtman 1996, Littlewood and Zhu 1996, Fernandez-Rossier and Tejedor 1997, Kim and Wolfe 1998). This type of structure is of special interest because (i) the barrier increases the exciton lifetime and avoids formation of biexcitons, (ii) from a theoretical point of view the electron and hole motions in the infinitesimally thin layers can be regarded as pure two-dimensional (2D) motions without any quantization along the direction perpendicular to the layers. Therefore the well-known mean-field theory of Bose–Einstein condensation of excitons in 3D case can be applied in pure 2D case without any problems. But, since electrons and holes are present in different layers, overlapping only at the interfaces, where their wave functions vanish, a dramatic decrease in the exciton binding energy occurs. For this reason the temperature at which the order parameter vanishes (i.e. the critical temperature for condensation) must be very small, because the critical temperature is related to the ionization of the Bose-condensed excitons with a small binding energy. Since in a quantum well the exciton binding energy increases with a decrease in quantum well widths, approaching four times the 3D effective Rydberg, the corresponding critical temperature, associated with the ionization of the excitons, must be higher. From this point of view, a single quantum well structure, in which the lifetime of excitons is long enough, should be more suitable for the appearance of the exciton condensed phase than the above-mentioned separated-layers structure.

In the present work, we address the problem of Bose–Einstein condensation of excitons in a single semiconductor quantum well. We take into account the fact that the electron and hole motions along the z direction (throughout this paper, we take the x-y plane to be the plane of

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confinement of the two-dimensional electron-hole system) are quantized into discrete levels due to the presence of a confinement potential along this direction. We will use a formal Green function treatment similar to the BCS theory of superconductivity. According this treatment the presence of Bose-condensed excitons modifies the single-particle Green functions, and therefore one has to consider the so-called 'anomalous' one-particle electron and hole Green functions. Those 'anomalous' Green functions vanish above a certain critical temperature, indicating that there is no longer a condensate of excitons in the system. In what follows we are interested in the case of quantum wells made from direct-gap semiconductors with non-degenerate and isotropic bands when the electron-hole pair is confined between two parallel, infinitely high potential barriers. With the perfect confinement approximation the dispersion laws for electrons $E_c(\boldsymbol{k}, \lambda)$ and holes $E_v(\boldsymbol{k}, \xi)$ are as follows (we set $\hbar = 1$):

$$E_c(\boldsymbol{k}, \lambda) = E_g + \frac{\boldsymbol{k}^2}{2m_e} + \frac{\pi^2\lambda^2}{2m_c L^2} \qquad E_v(\boldsymbol{k}, \xi) = -\frac{\boldsymbol{k}^2}{2m_v} - \frac{\pi^2\xi^2}{2m_v L^2}$$

where m_c and m_v are the electron and hole effective masses, E_g is the energy gap, $\boldsymbol{k}$ is a 2D wave vector and the quantum well has a thickness L. $\lambda, \xi = 1, 2, \ldots$ denote the quantum number of the states in the infinitely deep wells.

In what follows we assume that the excitons in a quantum well behave almost like weakly interacting Bose particles, and therefore one might expect that the Bose–Einstein condensation of excitons is possible. In this case the Fourier transforms of the inverse 'normal' and 'anomalous' one-particle Green functions are:

$$G_{cc}^{-1}(\boldsymbol{k}, \lambda, \lambda', \mathrm{i}\omega_m) = \delta_{\lambda\lambda'}\,[\mathrm{i}\omega_m - (E_c(\boldsymbol{k}, \lambda) - \mu_c)] \tag{1a}$$

$$G_{vv}^{-1}(\boldsymbol{k}, \xi, \xi', \mathrm{i}\omega_m) = \delta_{\xi\xi'}\,[\mathrm{i}\omega_m - (E_v(\boldsymbol{k}, \xi) - \mu_v)] \tag{1b}$$

$$G_{cv}^{-1}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m) = -\Sigma_{cv}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m) \tag{1c}$$

$$G_{vc}^{-1}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m) = -\Sigma_{vc}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m). \tag{1d}$$

Here G_{cc}^{-1}, G_{vv}^{-1} and G_{cv}^{-1}, G_{vc}^{-1} are the inverse 'normal' and 'anomalous' Green functions, respectively, μ_e and μ_v are the chemical potentials of the electrons and holes, and Σ_{ij} $(i, j = c, v)$ denote the corresponding mass operators (the mass operators Σ_{cc} and Σ_{vv} have been included in the effective masses in the corresponding dispersion relations). The symbol ω_m is denoted by $\omega_m = (2\pi/\beta)(m+1/2)$, $\beta = (k_B T)^{-1}$, k_B is the Boltzman constant, T is the temperature and $m = 0, \pm1, \pm2, \ldots$. The mass operators in the Dyson equations (1c) and (1d) can be written as a sum of a Hartree part and a screened Fock part. The Hartree term vanishes because of the global neutrality of the electron-hole system. In what follows we will extract from the mass operators only the screened static Fock terms $\Sigma_{cv}(\boldsymbol{k}, \lambda, \xi) = \Delta_{cv}(\boldsymbol{k}, \lambda, \xi)$ and $\Sigma_{vc}(\boldsymbol{k}, \xi, \lambda) = \Delta_{vc}(\boldsymbol{k}, \xi, \lambda)$. In this approximation equations (1c) and (1d) assume the forms:

$$G_{cv}^{-1}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m) = -\Delta_{cv}(\boldsymbol{k}, \lambda, \xi) \tag{1e}$$

$$G_{vc}^{-1}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m) = -\Delta_{vc}(\boldsymbol{k}, \xi, \lambda) \tag{1f}$$

The 'normal' $G_{cc}(\boldsymbol{k}, \lambda, \lambda', \mathrm{i}\omega_m)$,$G_{vv}(\boldsymbol{k}, \xi, \xi', \mathrm{i}\omega_m)$ and 'anomalous' $F_{cv}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m)$, $F_{vc}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m)$ one-particle Green functions can be obtained by solving the following set of equations:

$$\delta_{\lambda\lambda'} = \sum_{\lambda''} G_{cc}(\boldsymbol{k}, \lambda, \lambda'', \mathrm{i}\omega_m) G_{cc}^{-1}(\boldsymbol{k}, \lambda'', \lambda', \mathrm{i}\omega_m) - \sum_{\xi} F_{cv}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m)\Delta_{vc}(\boldsymbol{k}, \xi, \lambda') \tag{2a}$$

$$0 = -\sum_{\lambda'} G_{cc}(\boldsymbol{k}, \lambda, \lambda', \mathrm{i}\omega_m)\Delta_{cv}(\boldsymbol{k}, \lambda', \xi) + \sum_{\xi'} F_{cv}(\boldsymbol{k}, \lambda, \xi', \mathrm{i}\omega_m) G_{vv}^{-1}(\boldsymbol{k}, \xi', \xi, \mathrm{i}\omega_m) \tag{2b}$$

$$0 = \sum_{\lambda} F_{vc}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m) G_{cc}^{-1}(\boldsymbol{k}, \lambda, \xi', \mathrm{i}\omega_m) - \sum_{\xi'} G_{vv}(\boldsymbol{k}, \xi, \xi', \mathrm{i}\omega_m)\Delta_{vc}(\boldsymbol{k}, \xi', \lambda) \tag{2c}$$

$$\delta_{\xi\xi'} = -\sum_{\lambda} F_{vc}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m)\Delta_{cv}(\boldsymbol{k}, \lambda, \xi') + \sum_{\xi''} G_{vv}(\boldsymbol{k}, \xi, \xi'', \mathrm{i}\omega_m)G_{vv}^{-1}(\boldsymbol{k}, \xi'', \xi', \mathrm{i}\omega_m). \tag{2d}$$

The 'normal' phase of the system under consideration can be described by setting the non-diagonal parts of mass operator Δ_{cv} and Δ_{vc} equal to zero. Thus, Δ_{cv} and Δ_{vc} are the order parameters for the condensed phase. Using the static Fock terms, one can write the order parameters in the following forms:

$$\Delta_{cv}(\boldsymbol{k}, \lambda, \xi) = -\sum_{q}\sum_{\lambda',\xi'}\sum_{\omega_m} \frac{2\pi e^2}{\varepsilon_\infty |\boldsymbol{q} - \boldsymbol{k}|} f_{\lambda\xi'\xi\lambda'}(L|\boldsymbol{q} - \boldsymbol{k}|) F_{cv}(\boldsymbol{q}, \lambda', \xi', \mathrm{i}\omega_m) \tag{3a}$$

$$\Delta_{vc}(\boldsymbol{k}, \xi, \lambda) = -\sum_{\boldsymbol{q}}\sum_{\lambda',\xi'}\sum_{\omega_m} \frac{2\pi e^2}{\varepsilon_\infty |\boldsymbol{q} - \boldsymbol{k}|} f_{\lambda\xi'\xi\lambda'}(L|\boldsymbol{q} - \boldsymbol{k}|) F_{vc}(\boldsymbol{q}, , \xi', \lambda', \mathrm{i}\omega_m). \tag{3b}$$

Here the symbol $\sum_{\omega_m}$ denotes $\beta^{-1}\sum_{m=0,\pm1,\ldots} \ldots$. The function $f_{\lambda\xi'\xi\lambda''}$ is defined as follows:

$$f_{\lambda\xi'\xi\lambda'}(L|\boldsymbol{p}|) = \int_0^L \mathrm{d}z_1 \int_0^L \mathrm{d}z_2 \exp(-|\boldsymbol{p}| \cdot |z_1 - z_2|)\varphi_\lambda(z_1)\varphi_{\xi'}(z_2)\varphi_\xi(z_2)\varphi_{\lambda'}(z_1)$$

where

$$\varphi_\lambda(z) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\lambda\pi z}{L}\right).$$

In the set of equations (2) for the 'normal' and 'anomalous' one-particle Green functions one can observe the difference between the condensate we are studying, and this occurring in the case when the electrons and holes are in two different infinitesimally thin layers separated by a wide barrier material. In the case of a quantum-well structure one should take into account the composite nature of excitons, made up with two fermions, each one with different quantized motion along the direction perpendicular to the x-y plane. For this reason a complicated mixing of excitations will take place, unlike the above-mentioned case of two different infinitesimally thin layers. If one takes into account $\lambda = 1, 2, \ldots, n_1$ quantized electron states and $\xi = 1, 2, \ldots, n_2$ quantized hole states, then $n_1 + n_2$ poles for each of propagators G_{cc}, G_{vv}, F_{cv} and F_{vc} have to be considered.

It is impossible to solve exactly the set of equations (2) for arbitrary n_1 and n_2, and so we must introduce some approximation. We suppose that, when the number of electron–hole pairs in the well is small (the low density limit), one can take the right-hand side of the gap equations (3) in the lowest order in the density. In this case the 'anomalous' one-particle Green functions in the lowest order in density can be written in the form:

$$F_{cv}(\boldsymbol{k}, \lambda, \xi, \mathrm{i}\omega_m) = \frac{\Delta_{cv}(\boldsymbol{k}, \lambda, \xi)}{[\mathrm{i}\omega_m - (E_c(\boldsymbol{k}, \lambda) - \mu_c)][\mathrm{i}\omega_m - (E_v(\boldsymbol{k}, \xi) - \mu_v)]} + O(\Delta \cdot \Delta) \tag{4a}$$

$$F_{vc}(\boldsymbol{k}, \xi, \lambda, \mathrm{i}\omega_m) = \frac{\Delta_{vc}(\boldsymbol{k}, \xi, \lambda)}{[\mathrm{i}\omega_m - (E_c(\boldsymbol{k}, \lambda) - \mu_c)][\mathrm{i}\omega_m - (E_v(\boldsymbol{k}, \xi) - \mu_v)]} + O(\Delta \cdot \Delta). \tag{4b}$$

Defining

$$\psi_{\lambda\xi}(\boldsymbol{k}) \equiv \frac{\Delta_{cv}(\boldsymbol{k}, \lambda, \xi)}{E_c(\boldsymbol{k}, \lambda) - E_v(\boldsymbol{k}, \xi) - \mu^0_{exc}} \tag{5}$$

where $\mu^0_{exc} = \mu_e - \mu_v$ is the chemical potential of excitons (μ^0_{exc} in this approximation does not depend on the density), and by means of (3a) and (4a) one can obtain the following equation

for the function $\psi_{\lambda\xi}(\boldsymbol{k})$:

$$\left[E_g + \frac{\pi^2\lambda^2}{2m_cL^2} + \frac{\pi^2\xi^2}{2m_vL^2} - \mu^0_{exc} + \frac{\boldsymbol{k}^2}{2\mu}\right]\psi_{\lambda\xi}(\boldsymbol{k}) + \sum_{\lambda',\xi'}\sum_{\boldsymbol{q}} \frac{2\pi e^2}{\varepsilon_\infty |\boldsymbol{k}-\boldsymbol{q}|} f_{\lambda\xi'\xi\lambda'}(L|\boldsymbol{k}-\boldsymbol{q}|)\left[n_F\left(E_c(\boldsymbol{q},\lambda') - \mu_c\right) - n_F\left(E_v(\boldsymbol{q},\xi') - \mu_v\right)\right]\psi_{\lambda'\xi'}(\boldsymbol{q}) = 0 \tag{6}$$

where $\mu^{-1} = m_c^{-1} + m_v^{-1}$ is the exciton reduced mass and $n_F(x) = \left[\exp(\beta x) + 1\right]^{-1}$ is the Fermi function. The equation (6) is the familiar Wannier equation for an exciton with zero center-of-mass momentum in the infinitely deep well. One can solve (6) by expanding $\psi_{\lambda\xi}(\boldsymbol{k})$ into a basis $R_{n,m}(\boldsymbol{k}) = R_{n,m}(k,\vartheta)$ of the radial functions of a 2D hydrogen atom system (Shinada and Sugano 1966):

$$\psi_{\lambda\xi}(\boldsymbol{k}) = \sum_{n,m} C_{nm}(\lambda,\xi) R_{n,m}(k,\vartheta) \tag{7}$$

where $n = 0, 1, 2, \ldots$ is the principal quantum number, and for a given n, the angular momentum quantum number $m = 0, \pm1, \pm2, \ldots, \pm n$. $C_{nm}(\lambda,\xi)$ satisfies the following set of equations:

$$\left[E_g + \frac{\pi^2\lambda^2}{2m_cL^2} + \frac{\pi^2\xi^2}{2m_vL^2} - \mu^0_{exc} - E^{2D}_n\right]C_{nm}(\lambda,\xi) + \sum_{n',m'}\sum_{\lambda',\xi'}\sum_{\boldsymbol{k},\boldsymbol{q}} \frac{2\pi e^2}{\varepsilon_\infty|\boldsymbol{k}-\boldsymbol{q}|}\left(f_{\lambda\xi'\xi\lambda'}(L|\boldsymbol{k}-\boldsymbol{q}|) - \delta_{\lambda\lambda'}\delta_{\xi\xi'}\right)R^*_{n,m}(\boldsymbol{k})R_{n',m'}(\boldsymbol{q}) \times \left[n_F\left(E_c(\boldsymbol{q},\lambda') - \mu_c\right) - n_F\left(E_v(\boldsymbol{q},\xi') - \mu_v\right)\right]C_{n'm'}(\lambda',\xi') = 0 \tag{8}$$

where E^{2D}_n is the corresponding 2D-hydrogen atom energy. We expect to find all excitons condensed in the lowest excitonic state and so one can assume that $\lambda = \xi = 1$. Our next aim is to find how the chemical potential of excitons depends upon parameter L/a_0, where $a_0 = \varepsilon_\infty\mu^{-1}e^{-2}$ is the exciton Bohr radius. To do this we assume that the temperature $T = 0$ K. Then we take into account only the $\lambda' = \xi' = 1$ term on the left-hand side of (8) and use the variational method with a function

$$R_{1,0}(\boldsymbol{k}) = \sqrt{\frac{\pi}{2}}\left(\frac{4\beta}{a_0}\right)^2\left[\boldsymbol{k}^2 + \frac{4\beta^2}{a_0^2}\right]^{-3/2}. \tag{9}$$

The parameter β can be determined by maximizing the chemical potential μ^0_{exc} with respect to β. Thus we obtain the following equation for the chemical potential μ^0_{exc}:

$$\frac{E_g + \frac{\pi^2}{(L/a_0)^2}E_0 - \mu^0_{exc}(\beta)}{E_0} = -4\beta^2 + 128\beta^3\int_0^{+\infty} \mathrm{d}x \frac{f(xL/a_0)}{\left(x^2 + 16\beta^2\right)^{3/2}} \tag{10}$$

where $E_0 = \left(2\mu a_0^2\right)^{-1}$ is the effective exciton Rydberg and the function $f(x)$ is defined as follows:

$$f(x) = \frac{3x^2 + 8\pi^2}{x\left(x^2 + 4\pi^2\right)} - \frac{32\pi^4\left(1 - \exp(-x)\right)}{x^2\left(x^2 + 4\pi^2\right)^2}.$$

We have numerically maximized the expression (10) for the different values of the well thickness L/a_0 . Figure 1 shows the dimensionless chemical potential μ^0_{exc}/E_0, measured from the total ground-state energy $E_g + \frac{\pi^2}{(L/a_0)^2}E_0$ of the electron–hole pair in the well as a

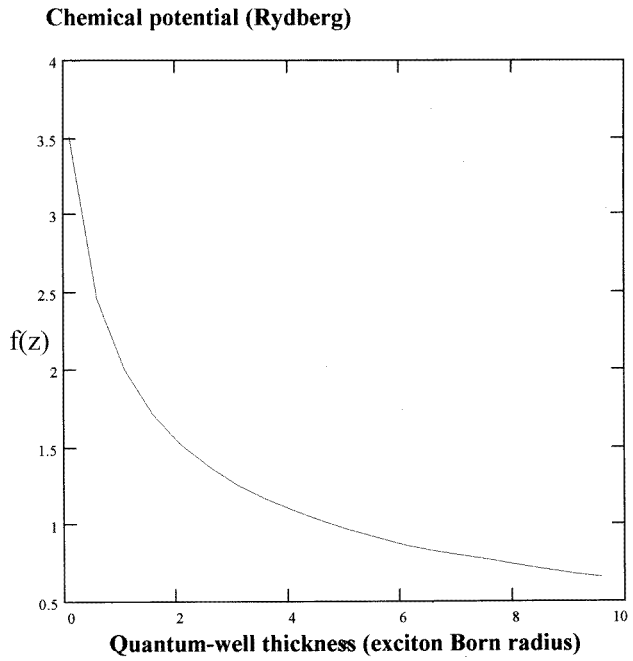

Figure 1. The calculated dimensionless chemical potential of excitons μ^0_{exc}/E_0 (E_0 is the 3D exciton Rydberg), measured from the total ground-state energy of the electron–hole pair in the well as a function of the dimensionless well thickness L/a_0 (a_0 is the 3D exciton Born radius).

function of the dimensionless well thickness L/a_0 . The chemical potential tends to $4E_0$ when L tends to zero. As can be seen, the two-dimensional behaviour of the chemical potential disappears very quickly: for $L/a_0 = 1$, $\mu^0_{exc} \approx 2E_0$. For $L > 4a_0$ the trial function $R_{1,0}$ leads to the chemical potential already smaller than E_0, and so our trial wave function is well suited for narrow well structures, but is not so good for a large L limit.

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