Dimensionality of exciton-state renormalization in highly excited semiconductors

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Renormalization of the band gap and exciton state in the presence of high-density electron-hole pairs is studied systematically for quasi-one-dimensional (q-1D), quasi-two-dimensional (q-2D), and three-dimensional (3D) systems. By introducing a universal measure of particle packing, it is shown that renormalization proceeds less effectively in lower dimensions. The exciton state disappears (Mott transition) due to the Coulomb-potential screening in the 3D system, the phase space filling in the q-1D system, and both of them in the q-2D system, although the screening is important at densities below the Mott density for every dimension.

Recently, much attention has been focused on confined semiconductor systems,[1] the research of which was initiated for quasi-two-dimensional (q-2D) electronic structures. This research is now being directed toward those of lower dimensions to search for new physics.[2] When these semiconductor systems are exposed to high excitation, which occurs, for example, in semiconductor lasers and nonlinear optical devices, their band gap and exciton energy levels are shifted (renormalized) due to the many-body effects of the injected electron-hole (e-h) pairs.[3-5] Several authors have compared the band-gap renormalization in the q-2D and three-dimensional (3D) systems.[6,7] However, to our knowledge, no systematic comparison has so far been made of the band gap and exciton state renormalization among systems of different dimensions. The purpose of this report is to discuss the energy renormalization for systems of different dimensions on the same theoretical basis and to clarify the effects of the various dimensions (dimensionality) on this phenomenon.

We employ two-band (electron and heavy-hole bands) approximation for simplicity. Moreover, for the q-1D and q-2D systems, we consider only the lowest subbands in these two bands. Under the assumption of static screening for the Coulomb potential, band-gap renormalization in q-1D system can be written as

$$\Delta(K)=-\sum_{\substack{K'\\ i=e,h}} f_i(K')V_s(K'-K) -\sum_{K'}[V_0(K'-K)-V_s(K'-K)]\ , \tag{1}$$

where the first term is the screened exchange energy and the second is the Coulomb-hole energy. Equation (1) is the q-1D version of equations derived previously for q-2D and 3D systems.[3-5] Here, $f_i(K)=1/(1+\exp\{\beta[E_i(K)-\mu_i]\})$ is the Fermi distribution function for $i=e$ (electron) and h (hole), where $E_i(K)=\hbar^2K^2/2m_i$ and $\beta=1/k_BT$. We employ the analytical form[8,9]

$$V_0(z)=\frac{e^2}{\varepsilon_r}\frac{a}{|z|+b}\ , \tag{2}$$

as the effective q-1D Coulomb potential in the real space between an electron and a hole, where a and b are parameters determined such that Eq. (2) accurately describes the numerically evaluated effective Coulomb potential in an actual q-1D system. Its Fourier transform is also known to have the analytical form

$$V_0(K)=\frac{2e^2a}{\varepsilon_r}G(bK)\ , \tag{3}$$

where

$$G(x)=\left[\frac{\pi}{2}-\mathrm{Si}x\right]\sin x-\mathrm{Ci}x\cos x\ . \tag{4}$$

Here, Six and Cix are the sine and cosine integrals,[10] respectively. The statically screened Coulomb potential is given by $V_s(K)=V_0(K)/\varepsilon(K)$ and the dielectric function $\varepsilon(K)$ by

$$\varepsilon(K)=1-V_0(K)2\sum_{\substack{K'\\ i=e,h}}\frac{f_i(K')-f_i(K'-K)}{E_i(K')-E_i(K'-K)}\ , \tag{5}$$

using random-phase approximation. Here, in the evaluation of Eq. (5), we replace the Fermi functions with Boltzmann functions for simplicity. In this way, we obtain a simple form of the dielectric function

$$\varepsilon(K)=1+\kappa G(bK)\sum_{i=e,h}\tfrac{1}{2}\phi\left[\hbar K\left[\frac{\beta}{8m_i}\right]^{1/2}\right]\ , \tag{6}$$

where $\kappa=4e^2a\beta N_1/\varepsilon_r$ is the q-1D screening wave number, N_1 is the q-1D e-h pair density (in units of cm^{-1}), and $\phi(x)$ is given by

$$\phi(x)=\frac{1}{2\sqrt{\pi}x}P\int_{-\infty}^{\infty}\frac{e^{-t^2}}{x-t}dt\ , \tag{7}$$

where P takes the principal value of the integration. This function is normalized so that $\phi(0)=1$. The exciton state is described by the homogeneous part of the Bethe-Salpeter equation[4]

$$\sum_{K'}H_{KK'}\varphi(K')=E\varphi(K)\ , \tag{8}$$

with the Hamiltonian

$$H_{KK'}=\left[E_g^0+\frac{\hbar^2K^2}{2\mu}+\Delta(K)\right]\delta_{KK'}$$
$$-[1-f_e(K)-f_h(K)]V_s(K'-K)\ , \tag{9}$$

using the statically screened Coulomb potential $V_S(K)$. Here, E_g^0 is the band gap in the absence of e-h plasma and $\mu=(m_e^{-1}+m_h^{-1})^{-1}$ is the reduced mass. The exciton energy can be obtained by minimizing the expectation value of the Hamiltonian in terms of the two-parameter (λ and σ) normalized variational wave function for the ground-state exciton proposed previously,[8]

$$\varphi(z)=\frac{\exp\left[-\sqrt{(z/\lambda)^2+\sigma^2}\right]}{\sqrt{2\sigma\lambda K_1(2\sigma)}}\ , \tag{10}$$

with its Fourier transform

$$\varphi(K)=\left[\frac{2\sigma\lambda}{K_1(2\sigma)}\right]^{1/2}\frac{K_1\left[\sigma\sqrt{\lambda^2K^2+1}\right]}{\sqrt{\lambda^2K^2+1}}\ . \tag{11}$$

Here, K_1 is the modified Bessel function.[10] The expectation value is primarily determined by the λ value chosen and is not very sensitive to σ.

Systems of higher dimensions can be treated similarly. Since the detailed calculations for higher dimensions are reported elsewhere,[3-5] we mention here only a few points. In the q-2D, the exciton wave function for the ground state is usually given by

$$\varphi(K)=\frac{\sqrt{8\pi\lambda^2}}{(\lambda^2K^2+1)^{3/2}}\ . \tag{12}$$

The Coulomb potential is expressed as

$$V_0(K)=\frac{2\pi e^2}{\varepsilon_r K}F(L_zK/\pi)\ , \tag{13}$$

where L_z is the well width and the form factor $F(x)$ can be expressed as the analytical form

$$F(x)=\frac{8}{\pi^2(x^2+4)}\left[\frac{\pi(3x^2+8)}{8x}-\frac{4(1-e^{-\pi x})}{x^2(x^2+4)}\right]\ , \tag{14}$$

for a q-2D system with infinite barrier height $[F(0)=1$ and $F(x)\sim 3/\pi x$ for $x\sim\infty$]. The exciton wave function for 3D is given by the hydrogenic wave function.

The above formulation is based on what Zimmermann[11] called the free virtual-state (FVS) approximation for the correlation term of the exciton energy. Recently, he pointed out that the inclusion of intraband and interband scattering terms could modify the exciton energy to some degree. Actually, he obtained the exciton energy twice that obtained by the FVS approximation at very low densities. At the current stage, we do not know how these scattering terms may modify the exciton energy in the high density region we are interested in, since there is no data in this region. However, we believe that the qualitative conclusion of this paper will not be changed by the inclusion of these terms.

It is clear from the above equations that two factors are responsible for energy renormalization: the screening effect for the Coulomb potential and the statistical carrier-filling effect [what we call the phase space filling (PSF) effect]. Here, we try to isolate these effects in order to study which one has the greatest impact on the renormalizing properties for each dimension. This can be done by simply plugging either $f_e(K)=f_h(K)=0$ (pure screening effect) or $\varepsilon(K)=1$ (pure PSF effect) into Eqs. (1) and (9). The results of this study will be shown later (Fig. 2).

We applied the above formulation to highly excited GaAs. The material parameters used were $m_e=0.067m_0$, $m_h=0.62m_0$, and $\varepsilon_r=10.8$: the potential barrier heights for the q-1D and q-2D are assumed to be infinite. The q-1D systems studied have L_x and L_y ranging from 50 to 130 Å and the q-2D systems have L_z ranging from 50 to 130 Å. We intentionally avoided very wide quantum structures [12] for which the higher subbands cannot be neglected in calculating the energy renormalization. The overall results can be summarized as follows: With increasing pair density N_d ($d=1$, 2, and 3), the exciton level E_x decreases together with the band gap $\Delta(0)=\Delta$, approaching each other. Finally, the exciton level gradually merges into the band gap (disappearance of the exciton state at the Mott transition) at a specific e-h pair density N_c (Mott density). This transition occurs at densities of 7.3×10^5 cm^{-1}, 3.1×10^{11} cm^{-2}, and 5.1×10^{16} cm^{-3} for the q-1D, q-2D, and 3D systems, respectively. These densities are independent of the size of the quantum structures. The energy renormalization values corresponding to the above densities are -65, -33, and -11 meV for the respective dimensions (the quantum-structure sizes used here are $L_x=L_y=50$ Å for q-1D and $L_z=50$ Å for q-2D). Energy renormalization appears to be correlated to the binding energy of the excitons because the former is approximately proportional to the latter ($\varepsilon_b=44$, 19, and 7 meV for the respective dimensions in the absence of e-h pairs). However, it may be difficult to compare the results more closely for different dimensions because the unit of density (a measure of e-h pair packing) differs between them.

Let us speculate on what could be a universal measure of particle packing. It must be a quantity that transcends the difference in dimensions in order to make a comparison possible. Several authors[6,7] have used r_s (for 3D, this is defined as the ratio of the Wigner-Seitz sphere's radius to the Bohr radius) to compare band-gap renormalization in the q-2D and 3D systems. Comparison using such a measure, however, does not seem to have a clear physical meaning because it is just like comparing the radius of a circle to that of a sphere. In addition, this measure does not show a reasonable dimensionality for the energy renormalization in the present study. Particle number in an exciton-volume r_s^{-d} ($d=1$, 2, and 3) reveals a reasonable dimension effect indeed, but we do not employ it since its physical implication is not clear either. We now introduce a measure that uses chemical potentials. Suppose there is a structure consisting of a semi-infinite 3D system and a q-1D system joined perpendicularly to it. Let the chemical potentials be μ_3 and μ_1 for 3D and q-1D systems, respectively. When $\mu_3>\mu_1$, the particles flow from 3D to q-1D, and vice versa. Then, the whole system approaches the state at which $\mu_3=\mu_1$ at which point there is no particle flow. From this, it seems natural to consider these systems to be equally packed by particles when there is no particle flow between them. Let us then define the effective density $N_{\rm eff}$ (in units of $\rm cm^{-3}$) as a universal measure of particle packing: $N_{\rm eff}$ is defined as the density in the 3D system at which the chemical potential has the same value as that in a given d-dimensional system. An arbitrary density N_d ($d=1$, 2, and 3) can be converted into $N_{\rm eff}$ by this procedure. N_3 is of course identical to $N_{\rm eff}$.

Figure 1 shows the calculated results of energy renormalization in the presence of e-h plasma, the shifts of the bandgap Δ, and the exciton state E_x as a function of the effective density. Both the screening effect and the PSF effect are considered in this calculation. The abscissa is normalized using the bulk exciton radius a_b and the ordinate is normalized using the exciton binding energy ε_b^0 for the respective dimensions in the absence of e-h plasma. The results of Fig. 1 do not depend on the size of the q-1D and q-2D systems and, therefore, can be regarded as intrinsic to the dimension, material, and temperature. The dimension effects are clear from Fig. 1. In 3D, the renormalized energy falls relatively quickly with increases in the pair density. This curve becomes more gradual as the dimension lowers. In other words, a higher $N_{\rm eff}$ is required in lower d systems to attain a certain energy shift (in its ε_b^0 normalized form). The lower efficiency of energy renormalization may be related to the conjecture that the Coulomb potential is less effectively screened by the e-h plasma in lower d systems.[5] Moreover, it is known that even a very weak attractive potential creates a bound state in the q-1D and q-2D systems, whereas it does not in the 3D system.[13] Thus, the persistent survival of the exciton state in low d systems may be partly the cause of the low efficiency of energy renormalization. These predictions will be clarified in following studies.

Figure 2 shows the exciton binding energy as a function of the effective density for the (a) q-1D, (b) q-2D, and

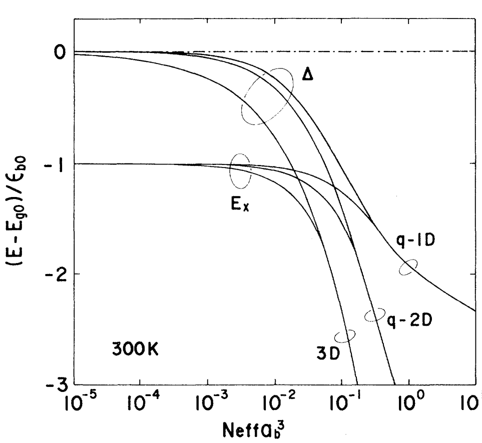

FIG. 1. Band gap Δ and exciton state E_x as functions of the effective density $N_{\rm eff}$. The density is normalized using the bulk exciton radius a_b and the energy using the exciton binding energy ε_b^0 in the respective dimensions in the absence of e-h plasma.

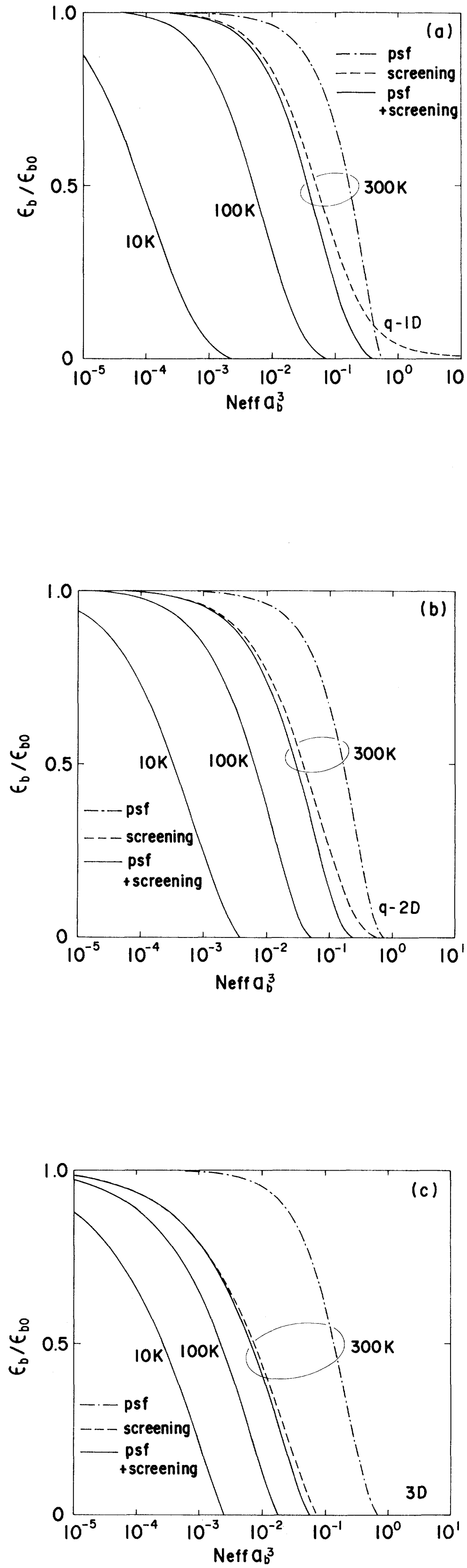

FIG. 2. Exciton binding energy ε_b as a function of the effective density $N_{\rm eff}$ for (a) q-1D, (b) q-2D, and (c) 3D systems.

(c) 3D systems. The solid lines indicate the results obtained from Fig. 1 using $\varepsilon_b = \Delta - E_x$: these include both the screening and the PSF effects. The dashed lines denote results obtained by considering only the screening effect and the dash-dotted lines are for only the PSF effect. With the increase in N_{eff}, the binding energy decreases and tends toward zero, which implies a disappearance of the exciton state (Mott transition). At densities below the Mott density (N_c), the screening effect is primarily responsible for the decrease in binding energy for every dimension. This effect varies depending on the dimension. In contrast to this, the PSF effect is far less influential on the ε_b decrease at densities below N_c. This is true especially in higher dimensions. Moreover, the ε_b renormalization due to this effect is found to exhibit nearly the same behavior irrespective of the dimensions. This is a reasonable result because N_{eff} is fundamentally a measure of particle packing in the K space. In the vicinity of the Mott transition, however, the situation is entirely different among the different dimensions. In the 3D system, the screening effect is still a main contributor to exciton-state disappearance. In the q-1D system, however, the PSF effect becomes dominant in this transition. Note that the exciton state continues to exist even at higher densities for the q-1D system under the condition that only screening is effective. In the q-2D system, both screening and PSF are responsible for the disappearance of the exciton state.

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