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Many-body effects on the luminescence spectrum of modulation-doped quantum wells

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The luminescence spectrum of modulation-doped quantum wells is investigated theoretically with regard to the many-body effects caused by the extra conduction electrons. In the zero-temperature limit vertex corrections are shown to be unimportant, so that the emission frequencies are determined by the self-energies of the valence-band holes and the conduction-band electrons. Calculations of the self-energies are carried out perturbationally, using the plasmon-pole approximation for the dielectric function. The electron- and hole-energy levels are also calculated self-consistently by local density-functional theory. The results of both theories agree satisfactorily with each other over a large range of conduction electron densities and explain recent experiments [Pinczuk *et al.*, Solid State Commun. **50**, 735 (1984)].

Modulation-doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells are well suited for the study of electron correlation effects because of the very high mobility of their conduction-band carriers.[1] Recently, optical experiments have revealed a reduction of the band gap in these systems with respect to the bulk GaAs,[2] which is a nice example of an intrinsic many-body effect. The related band-gap shrinkage in heavily doped semiconductors,[3] is, in contrast, affected significantly by the strong perturbation from the ionized dopants.[4–6] In the present Rapid Communication we will discuss the theory of the luminescence spectrum of modulation-doped quantum wells. Numerical results for the renormalization of the emission frequencies in modulation-doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells are compared with the experiment.[2]

The cross section for spontaneous light emission $d\sigma^{\rm em}/d\omega d\Omega$ is determined by Fermi's golden rule, assuming thermal quasiequilibrium of the excited carriers prior to recombination. In sufficiently perfect samples the luminescence is dominated by direct electron-hole recombinations in the quantum well, so that the cross section reads

$$\frac{d\sigma^{\rm em}}{d\omega d\Omega}(\omega)=|M|^2\{\exp[(\hbar\omega-E_g-\mu_a-\mu_b)/k_BT]-1\}^{-1}\times\sum_{kk'}\frac{2}{\pi}\,{\rm Im}[\mathcal{G}_{ab}(\mathbf{k},\mathbf{k}';\hbar\omega-E_g-\mu_a-\mu_b)]\,, \tag{1}$$

where $\mathcal{G}_{ab}(\omega)$ is the analytic continuation of the Fourier transform of the electron-hole two-particle Green's function $\mathcal{G}_{ab}(\tau)$ to the real axis. μ_a and μ_b are the chemical potentials of the electron and hole systems relative to the band edges of the bulk material of the quantum well (GaAs). The fundamental energy gap of the bulk is denoted by E_g. The matrix element M will not be considered any further, since we are not interested here in absolute intensities. The energy dispersion of conduction-band electrons and valence-band holes is taken to be positive.

Using perturbation theory many-body effects on $\mathcal{G}_{ab}$ may be separated into the renormalization of the electron and hole lines by the self-energies and the so-called vertex part. A general treatment of the vertex part which describes the interaction between the electron and hole under consideration is complicated. However, for not too high intensity of the photoexcitation radiation the hole density in modulation-doped quantum wells is small compared with the conduction-electron density. In this case the vertex part may be neglected for the following reason. At zero temperature and for a vanishing number of holes luminescence originates exclusively from the annihilation of electron-hole pairs at $\mathbf{k}=\mathbf{k}'=\mathbf{0}$. Any scattering of this pair into a higher momentum state is energetically unfavorable, since by phase space occupation an energy gap of the order of the conduction-electron Fermi energy has to be surmounted.

The intuitive result can be verified in the ladder approximation for the vertex part and the quasiparticle pole approximation for the one-particle Green's functions. Assuming, for example, a screened Coulomb interaction $\langle V\rangle$ independent of $\mathbf{k}$ and ω, we get

$$\lim_{T\to 0;N_b\to 0}\frac{d\sigma^{\rm em}}{d\omega d\Omega}(\omega)=|M|^2N_b\delta(\hbar\omega-E_g-\tilde{\epsilon}_0^a-\tilde{\epsilon}_0^b)\times\left[1+\langle V\rangle\sum_{k>k_f}\frac{1}{\tilde{\epsilon}_k^a-\tilde{\epsilon}_0^a+\tilde{\epsilon}_k^b-\epsilon_0^b}\right]^{-2} \tag{2}$$

to the lowest order in the number of holes N_b. $\tilde{\epsilon}_k^a$ and $\tilde{\epsilon}_k^b$ are the renormalized quasiparticle energies of the electrons and holes, respectively, and k_f is the Fermi wave vector of the conduction electrons. The shift of the luminescence frequency is thus given simply by the sum of the renormalized quasiparticle energies at the top of the valence band and the bottom of the conduction band, as assumed without discussion in previous approaches to the problem in heavily doped semiconductors.[3–7] The second factor in Eq. (2) renormalizes the emission intensity only. An artifact of the assumption of the δ-function electron-hole interaction is the logarithmic divergence of the sum over the wave vector in Eq. (2). However, the discussion is readily generalized to the case of wave-vector-dependent potentials where this problem does not arise. The above arguments may be extended to the elastic scattering from impurities, which is of interest for heavily doped semiconductors. The neglect of the imaginary part of the self-energy might be less justified in this case, however.

In the following we will discuss the energy shift by two independent approaches in order to gain some idea of the

quality of the approximations. On one hand, the self-energies are calculated explicitly for a two-dimensional system. The finite width of the quantum well is taken into account by weakening the Coulomb interaction by form factors[8,9] obtained from variational wave functions for the electrons and holes confined to the well. The use of variational wave functions can be avoided on the other hand by local density-functional theory[10] which allows for a numerically exact treatment.[11] Exchange or correlation is taken care of in this case by the use of effective one-particle potentials which are parametrized on the basis of the interacting three-dimensional electron gas. In both cases the plasmon-pole approximation[12] to the dielectric function has been chosen to calculate the electron correlation, since it combines computational simplicity with satisfactory accuracy.[7] We adopt the values 0.068 and 0.4 for the effective masses of electrons and holes (in units of the free electron mass) and 12.9 for the dielectric constant.

The real part of the self-energies for two-dimensional systems is calculated following Ref. 9. The screening of the bare Coulomb interaction is described by using a plasmon-pole approximation to the dielectric function of the two-dimensional electron gas. The form factors are determined by the envelope wave functions of the confined electrons and holes perpendicular to the interface which are represented here by single Gaussian wave functions. Form factors and energy expectation values can be expressed analytically. The self-consistent model for the electron wave function is then easily determined variationally in the Hartree approximation, while the hole wave function has to be optimized in the field of the conduction-electron charge density.

The eigenvalues of the Kohn-Sham self-consistent equations for the inhomogeneous electron gas[10] may be used as an approximation to the required one-particle excitation energies.[13] Electron-gas exchange-correlation potentials in conveniently parametrized forms are abundant in the literature. Here, the Gunnarson-Lundqvist potential[14] is used, which is based on calculations within the plasmon-pole approximation. The exchange-correlation potential for the hole system μ_{xc}^{b} is equal to the self-energy at $\mathbf{k}=\mathbf{0}$ of a positively charged particle in a three-dimensional electron gas. We have calculated this quantity in the plasmon-pole approximation recommended in Ref. 12. For equal masses our results agree with those from the random-phase approximation (RPA) calculations of Ref. 15 within about 3%. In GaAs the mass ratio is $m_a/m_b \cong 0.068/0.4 = 0.17$ which modifies the self-energy considerably. With an accuracy of about 2% over a large range of densities the following formula reproduces the calculations (in effective rydberg units):

$$\mu_{xc}^{b}(r_s) = -2[\sqrt{\pi\alpha r_s}(1 + Ar_s^{1/4} + Br_s^{1/8})]^{-1}, \quad (3)$$

where r_s is the electron-gas density parameter, $\alpha = (4/9\pi)^{1/3}$, $A = 1.26$, and $B = -0.58$. A is determined by the large-r_s expansion of the plasmon-pole self-energy and B is a fitting parameter. Similar calculations for the self-energies of holes exist for bulk GaAs.[7] The results are not strictly comparable, however, since contrary to the bulk calculations the coupling between heavy and light holes should be neglected in narrow quantum wells.

The numerical results obtained by both methods are summarized in Figs. 1–3. The calculations have been carried out for a width of 250 Å of the GaAs layer and an alloy parameter $x = 0.12$. Using Dingle's rule[16] this corresponds to conduction-band (valence-band) potential-barrier heights of 125 (22) meV. The curves labeled "Hartree" show the energies obtained in the Hartree approximation by both methods. The density-functional theory may be considered in this approximation as a numerically exact reference. The curves labeled "many-body" display the results which are obtained by including the self-energies and exchange-correlation potentials, respectively.

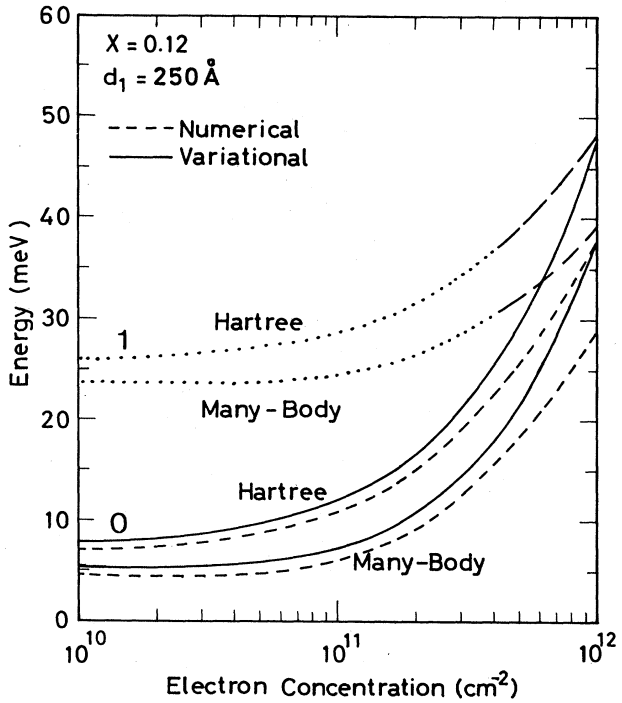

FIG. 1. Subband energies of conduction electrons in modulation-doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells (0—first subband; 1—second subband). The dotted line indicates unoccupied levels. The curves labeled "Hartree" represent the results of calculations in the self-consistent Hartree approximation [continuous curve —variational (Gaussian) wave function; dashed curve—numerical wave function]. The Hartree results are modified by exchange correlation as shown by the curves marked "many body" (continuous curve —self-energy added; dashed curves—self-consistent results using a local exchange-correlation potential, Ref. 14).

The agreement of the results of the variational method in the Hartree approximation with the corresponding ones of density-functional theory is at low densities a direct measure of the quality of the model wave function. In this case the deviations of the electron energy levels (Fig. 1) are solely due to the lack of flexibility of the single Gaussian-type envelope function. The wave function of the hole is well described by a single Gaussian, as can be judged from Fig. 2. At high densities the second electron subband becomes occupied, but with a single variational wave function only one subband can be formed. The lack of occupation of the second subband in the variational method at high densities increases the difference between the computed energy levels of the conduction electrons (Fig. 1). On the other hand the energy levels of the hole system become too low in the variational calculation (Fig. 2), because the Hartree potential for

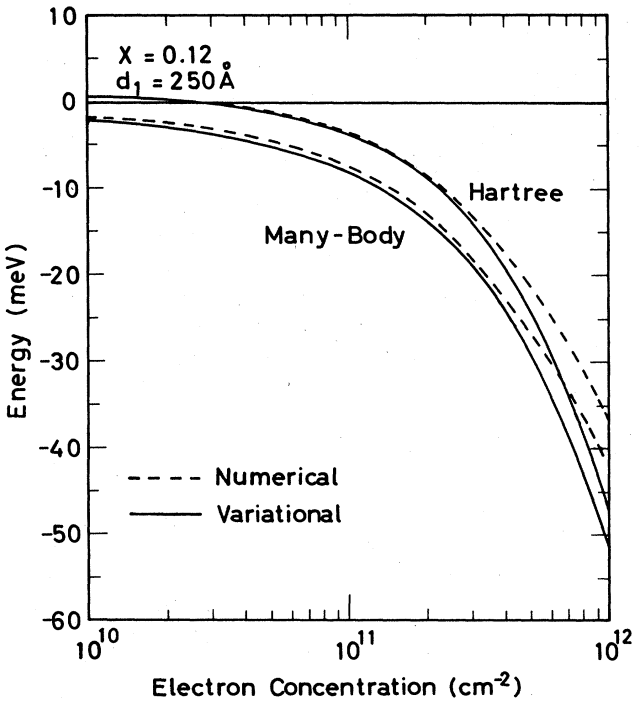

FIG. 2. Energies of the first subband of valence-band holes in modulation-doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells. The curves labeled "Hartree" display the results for a hole in the Hartree potential of the conduction electrons (cf. Fig. 1) [continuous curve—variational (Gaussian) wave function; dashed—numerical wave function]. The Hartree results are modified by exchange correlation as shown by the curves marked "many-body" [continuous curve—self-energy added; dashed curve—self-consistent results using the local exchange-correlation potential Eq. (3)].

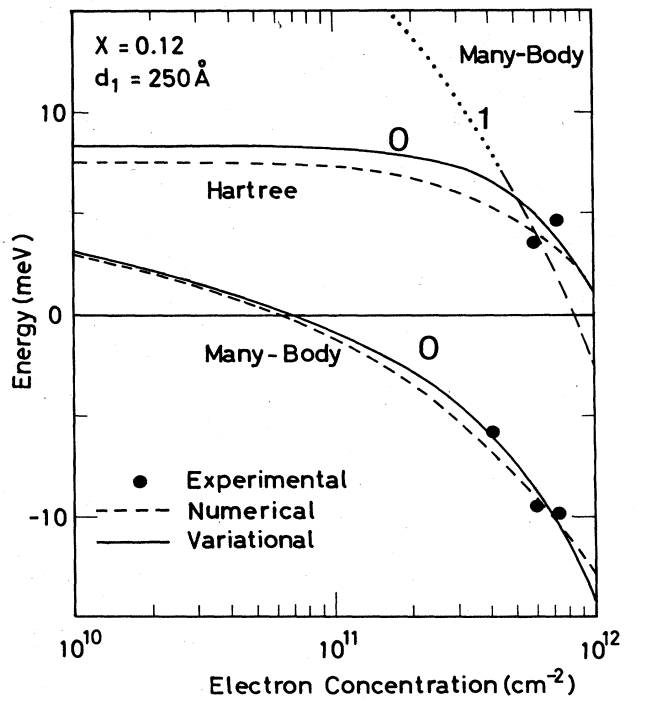

FIG. 3. Energy shifts of the luminescence radiation in modulation-doped GaAs-$Ga_{1-x}Al_xAs$ quantum wells relative to the energy gap in bulk GaAs (0—transitions between the first subbands; 1—transitions between the second subband of the conduction electrons and the first subband of the valence-band holes). The results are obtained by adding those of Figs. 1 and 2. The second electron subband is not occupied for the densities corresponding to the dotted line. The filled circles indicate the experimental results (Ref. 2) relative to the band gap of bulk GaAs of 1.519 eV.

the holes from the conduction electron density of the Gaussian wave function is too attractive. In the sum of electron and hole energies (Fig. 3), which amounts to the desired line shift, the errors thus cancel to a large extent. In the Hartree approximation the errors are less than 1 meV over the whole range of densities considered.

The many-body shifts computed by both methods are remarkably similar. The lowering of the energy levels is practically the same for the electrons (Fig. 1), while in case of the holes density-functional theory predicts slightly higher subband energies (Fig. 2). If many-body effects are considered the computed modifications of the energy gap turn out to be practically identical for both methods.

In Fig. 3 the experimental result is indicated in the form of dots which correspond to slightly lower energies than the peak positions of the main emission lines.[2] [Note that the alloy parameter of the low-density sample ($x = 0.23$) differs somewhat from the others and from the calculations.] In the present theory the transitions from the second subband are forbidden. The experimentally observed emissions point to unknown imperfections of the quantum wells which add some uncertainty to the quantitative interpretation of the data. Still, the agreement between experiment and theory is rather satisfactory, also for the transitions from the second subband. It would be desirable to have more experimental results available to be able to corroborate the trends in the calculations for a larger spread of sample parameters.

In conclusion, we find a generally good agreement between the results of the different methods and between calculations and the available experimental data. It is expected that by changing the charge density in modulation-doped quantum wells it is possible to vary the band gap in these systems over several meV relative to the energy gap of bulk GaAs.

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