Excitons in the quasi-two-dimensional electron gas

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The response of modulation-doped semiconductor quantum wells to a band-gap light field is discussed with special attention paid to excitons and screening. Absorption and luminescence spectra are calculated in a mean-field approximation, taking into account the confinement and finite mass of the particles, finite temperatures, and external magnetic fields. Bound excitonic states are found to dominate the low-temperature luminescence spectra for densities up to $\simeq 10^{11}$ cm^{-2}. At higher densities the excitonic state can be recovered by applying a magnetic field. The reappearance of the excitonic state is accompanied by an abrupt blueshift and increased oscillator strength of the luminescence. An efficient method to solve the zero-field Bethe-Salpeter integral equation in two dimensions is based on the application of a small auxiliary magnetic field.

I. INTRODUCTION

Traditionally the two-dimensional (2D) electron gas has been investigated mainly by transport experiments, which led to the discovery of the integer and fractional quantum Hall effect.[1] Optical spectroscopy can still yield additional and complementary information. Recent attempts to learn about the nature of the ground state in the regimes of the fractional quantum Hall effect and Wigner crystal by magnetoluminescence spectroscopy have attracted a lot of interest.[1,2] Theory has not been able to follow suit, however, and a satisfactory description of the optical properties of this strongly correlated electron system does not yet exist.[3] The difficulties are caused by the electron-hole correlations, i.e., the excitonic vertex correction, not to mention hole relaxation dynamics and related problems. Here it is assumed that the electron gas can be described by an ensemble of single determinants, taking into account many-electron effects only by renormalizing the single-particle energies and screening the electron-hole interaction, thus from the outset discarding any effects due to fractional quantization. Even in this simple approximation a theoretical prediction of the optical properties is by no means a trivial task. Conversely, it can be tricky to draw conclusions about the ground state of the system from the experimental luminescence and absorption spectra. The present study is partly motivated by the belief that a better understanding of the optical processes at zero magnetic fields and in the integer quantum Hall regime will be helpful in disentangling the effects of strong electron correlations on optical spectra.

In the limit of an infinite hole mass the problem becomes similar to that of x-ray core-hole spectra, which have been studied thoroughly in the past.[4] With a static, separable model potential for the screened electron-hole interaction "exact" solutions have been found.[4] These results are directly relevant for quantum wells in which the hole is localized.[5] Most calculations with realistic interactions have been carried out in the ladder approximation of the vertex correction[6] [Fig. 1(a)], which is accurate when the interaction potential is sufficiently small compared to the Fermi energy.[4] Mahan's[6] seminal work on highly doped bulk semiconductors has been extended to modulation-doped quantum wells,[7] to obtain the luminescence spectrum of a strictly 2D system and a localized hole,[8] and absorption spectra for 2D (Ref. 9) and quasi-2D (Ref. 10) systems. The main results are enhancements of the oscillator strength at the absorption edge, often referred to as "Fermi-edge singularity."

The effects of free carriers on bound excitonic states in quantum wells have been discussed in the low-density limit by Schmitt-Rink, Chemla, and Miller.[7] Exciton effects on the luminescence energy have been shown to be quenched at sufficiently high densities when the hole is allowed to recoil.[11] In other mean-field theories for high doping densities[6-10] bound states were discarded in order to simplify the numerical treatment of the problem. A computational method for a mean-field treatment of bound and scattering states on equal footing is desirable, since the former are expected to play important roles at lower electron densities.

In spite of the experimental efforts directed at the effects of magnetic fields on the optical properties,[1,2] theorists have maintained a rather low profile. Employ-

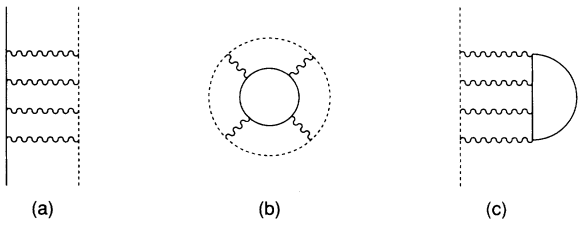

FIG. 1. Representative diagrams of the mean-field or ladder approximation in the present theory: (a) electron-hole Green's function, (b) thermodynamic potential, and (c) hole Green's function as used for the normalization of the luminescence intensity. The full and dashed lines denote the electron and hole single-particle Green's functions, respectively, and the wavy lines represent the screened Coulomb interaction.

ing the magnetic-field-dependent self-energy of the quasi-2D electron gas proposed by Ando and Uemura,[12] Katayama and Ando,[13] and Uenoyama and Sham[14] explained oscillations of the luminescence energy as a function of magnetic field[15] as a modulation of the band-gap renormalization. Two recent papers attempt to generalize the theory for the core-hole spectra to include the effects of the finite mass of the hole in semiconductors,[16,17] although the appeal of being "exact" treatments of the electron-hole correlations had to be sacrificed.

The analogy between the process of the recombination of a hole in an electron gas and the annihilation of positrons in a metal should be noted here. The latter has captured the interest of many-body theorists for quite some time.[18–20] There are differences concerning the quantities which are usually measured, i.e., energy-resolved luminescence spectrum vs momentum-resolved angular correlation of the positron annihilation radiation. The excitonic bound states discussed here correspond to (quasi)positronium states in low-density metals, the existence of which is being debated.[20] I am not aware of experimental studies of positron annihilation in simple metals at low enough density to settle the positronium problem. In quantum wells, on the other hand, the density can be freely adjusted by the doping level, and theoretical predictions are open to experimental verification. Also, because of the enhancement of excitonic effects by the reduced dimensionality and the strong temperature and magnetic-field effects, modulation-doped quantum wells are better suited for a study of many-body effects.

In the present paper the optical properties of modulation-doped quantum wells are investigated on a mean-field level. A realistic Coulomb interaction and a magnetic-field-dependent screening function are taken into account in calculating absorption and luminescence spectra. For the latter, surprising results are found which are a direct consequence of the bound states and the finite hole mass. The present paper is a final report of a project, some results of which have been reported previously. In Refs. 21–23 magnetoabsorption and luminescence spectra have been obtained in the Hartree-Fock approximation, i.e., neglecting screening effects. An exciton instability in the Hartree-Fock theory was reported first in Ref. 23. Though qualitatively correct, results of Hartree-Fock theory have subsequently been found to be strongly modified by screening.[24] Since a zero-field screening function has been used, the results of Ref. 24 were limited to small magnetic fields, however. Some results obtained with magnetic-field-dependent screening[12] have been presented in Ref. 25. The optical properties of modulation-doped quantum wells are quite different from those of highly excited quantum wells containing neutral electron-hole plasmas, which are discussed elsewhere.[22,26,27]

Expressions for the absorption spectra are given in Sec. II. They account for the effects of confinement, magnetic fields, finite temperatures, and excitonic bound states. In the weak-excitation limit the luminescence intensity vanishes with the number of holes and must therefore be treated with care. As shown in Sec. III, the relevant quantity is the luminescence intensity divided by the number of optically active holes. The results of numerical calculations are presented in Sec. IV. The validity of the mean-field theory is critically discussed in Sec. V. The experimental evidence is reviewed in Sec. VI and the conclusions are summarized in Sec. VII.

II. ABSORPTION SPECTRA OF MODULATION-DOPED QUANTUM WELLS

The optical properties, i.e., the linear response to a weak photon probe, can be expressed in terms of the two-particle electron-hole Green's function,[28,29] which is determined by the so-called Bethe-Salpeter integral equation. Here we are interested in the electron-hole Green's function for modulation-doped quantum wells, also in the presence of magnetic fields. Very small fields do not cause any physical effects, but provide a convenient numerical discretization scheme, which is preferable to a momentum-space sampling, because Landau levels are equidistant in energy. One has to pay for these advantages by complicated Coulomb matrix elements. However, as shown in the Appendix, these do not cause serious problems.

Conventional perturbation theory can be applied to calculate the optical spectra by assuming thermal quasiequilibrium at given electron and hole densities ρ_e and ρ_h. Let us consider a quantum well with intersubband spacings which are large enough to disregard higher subbands and apply a magnetic field normal to the interfaces. A two-subband model of parabolic bands is adopted in the following, and the small g factors of electrons and holes are assumed to be zero; i.e., spin-splittings are neglected. The theory of the optical spectra of three-dimensional systems and in the absence of magnetic fields is reviewed in Ref. 28. By a straightforward generalization the absorption spectra for the present system are found to be proportional to

$$I^{\mathrm{abs}}(\hbar\omega)=\frac{1}{\pi l^2}\frac{1}{\pi}\mathrm{Im}\sum_{m,n}G_{eh}(m,n;\hbar\omega-i\delta)\ , \tag{1}$$

where $l=\hbar/eB$ is the magnetic length and m and n are Landau-level indices. The electron-hole Green's function in the mean-field approximation is conveniently calculated by making use of a biorthogonal expansion described by Stolz,[29] which has to be modified to include the confinement and magnetic fields normal to the interfaces. The matrix elements are related to the exchange integrals which modify the magnetoplasmon dispersion in the quasi-2D electron gas.[30] The details are tedious, and will not be spelled out here. The final equations for the optical spectra at arbitrary particle densities (but in the absence of electron-hole pairing[26]) are summarized below in a form which is readily computed numerically. The sum over states in the electron-hole Green's function becomes

$$\sum_{m,n}G_{eh}(m,n;\hbar\omega)=\sum_{i}\frac{\mathrm{sgn}[\lambda_i-\mu_e-\mu_h]}{\hbar\omega-\lambda_i}\times\left|\sum_{n}\phi_i(n)\sqrt{|F(n)|}\right|^2\ , \tag{2}$$

where ϕ_i (assumed normalized) and λ_i are the solutions of the eigenvalue problem

$$\sum_n \{E(m)\delta_{mn} - \mathrm{sgn}[F(m)]\sqrt{|F(m)|} \times V_{eh}^S(m,n)\sqrt{|F(n)|}\}\phi_i(n) = \lambda_i \phi_i(m) , \quad (3)$$

and μ_e and μ_h are the (quasi)chemical potentials of electrons and holes. The factors

$$F(n) = 1 - f_e(n) - f_h(n) , \qquad f_a(n) = \frac{1}{e^{\beta[E_a(n)-\mu_a]}+1}, \quad \beta = \frac{1}{k_B T} \quad (4)$$

take account of the phase-space occupation of states with quasiparticle energies

$$E_a(n) = E_a^{\mathrm{sub}} + \frac{eB\hbar}{m_a}(n+\tfrac{1}{2}) + \Sigma_a(n) \quad (5)$$

and

$$E(n) = E_e(n) + E_h(n) . \quad (6)$$

The third term on the righthand side of Eq. (5) is the self-energy of particle type of a, which is considered here in two approximations. The quasistatic approximation[28,14] is computationally very convenient, but the self-energies are not treated on the same footing with the vertex correction,[27] which leads to a wrong limiting behavior at high magnetic fields.[31] Results will therefore also be presented in the plasmon-pole approximation to the self-energy,[29,13] which is computationally considerably more involved, but which reduces correctly to the Hartree-Fock results in the high-magnetic-field limit.[27]

The matrix elements of the bare (superscript 0) and screened (superscript S) Coulomb potential matrix elements read as follows:

$$V_{ab}^{0/S}(n,m) = \int \frac{dq}{2\pi} q V_{ab}^{0/S}(q) |J_{nm}(q)|^2 , \quad (7)$$

where

$$J_{nm}(q) = \left[\frac{N!}{M!}\right]^{1/2} e^{-l^2q^2/4}(lq/2)^{M-N} \times L_M^{M-N}(l^2q^2/2) \quad (8)$$

in terms of the associated Laguerre polynomials $L_n^{(\alpha)}$ and $M = \max(m,n)$, $N = \min(m,n)$.

$$V_{ab}^0(q) = \frac{2\pi e^2}{\kappa q} \int dz\, dz' |\xi_a(z)|^2 |\xi_b(z')|^2 e^{-q|z-z'|} \quad (9)$$

is the absolute value of the bare Coulomb potential for quasi-2D systems, where κ denotes the static dielectric constant of the intrinsic bulk semiconductor. The spatial integrals reflect the softening of the Coulomb interactions compared to the strictly 2D limit. In general the electron and hole subband envelope functions ξ_e and ξ_h are different, and a dielectric screening matrix needs to be introduced:

$$\epsilon_{ab}(q) = \delta_{ab} - V_{ab}^0(q)\Pi_b(q) , \quad (10)$$

where $\Pi_{e(h)}$ denote the static polarizabilities of electron and hole systems. In terms of the inverse dielectric matrix we finally obtain

$$V_{ab}^S(q) = \sum_c [\epsilon^{-1}(q)]_{ac} V_{cb}^0(q) . \quad (11)$$

The subband envelope functions are chosen to be Gaussians with half-widths which minimize the total Hartree energy.[11] The form factors can modify the results qualitatively compared to the strictly 2D system.[22] On the other hand, it was found to be a good approximation to set the form factors F_{ee} and F_{hh} equal to F_{eh}, which simplifies computations considerably, e.g., the dielectric matrix becomes diagonal. In the numerical results presented here this approximation is in effect. The evaluation of the integrals in Eq. (7) for Gaussian envelopes is discussed in the Appendix.

Finally, the static polarizabilities $\Pi_{e(h)}$ in Eq. (10) have to be calculated. When the Landau-level spacing is sufficiently smaller than the single-particle lifetime broadening, the polarizabilities are not modified from the zero-field results. The zero-field temperature-dependent Lindhard screening[32] is adopted in this case. The singularities in the polarizabilities at finite magnetic fields are treated according to Ando and Uemura[12] by introducing a small impurity potential. The level broadening is calculated in the self-consistent Born approximation. Only the low-temperature limit is considered here, where $1/\beta$ is much smaller than the level broadening. The high-temperature limit is discussed in Ref. 27. The intra-Landau-level screening in magnetic fields is obtained at the cost of an adjustable zero-field broadening parameter Γ_a which characterizes the quality of the sample. The magnetic-field-dependent broadening of the Landau levels is then $\Gamma_B = \sqrt{2eB\hbar\Gamma_a/m_a\pi}$. Γ_B (not Γ_a) is taken to be identical for electrons and holes, which is consistent with the neglect of the difference in the form factors.

III. LUMINESCENCE SPECTRA

Formally, the photoluminescence is obtained from the absorption spectrum Eq. (1) as[28]

$$I^{\mathrm{lum}}(\hbar\omega) = I^{\mathrm{abs}}(\hbar\omega)/(e^{\beta(\hbar\omega-\mu_e-\mu_h)}-1) . \quad (12)$$

In highly excited semiconductors above the plasma condensation temperature,[26] the luminescence spectrum is easily obtained from the absorption spectra discussed in the preceding section. In the low excitation limit the density of the minority carriers (without loss of generality assumed in the following to be the holes) ρ_h tends to zero, however. The luminescence intensity becomes vanishingly small relative to the absorption and Eq. (12) cannot be used straightforwardly. It will be shown below that the total hole density can be classified as optically active and inactive:

$$\rho_h = \rho_h^{\mathrm{act}} + \rho_h^{\mathrm{inact}} . \quad (13)$$

A proper measure of the *oscillator strength* associated with a luminescence line is the ratio

$$F^{\rm lum}(\hbar\omega)=\lim_{\rho_h\to 0} I^{\rm lum}(\hbar\omega)/(\pi l^2\rho_h^{\rm act}) , \tag{14}$$

which is well behaved, though its evaluation requires additional effort.

The hole number can be obtained from the hole (single-particle) Green's function, which should be calculated in an approximation that is consistent with the ladder approximation for the two-particle Green's function or equivalently, as the derivative of the thermodynamic potential Ω with respect to the hole chemical potential.[33] By cutting a hole line of Ω in the ladder approximation [Fig. 1(b)], a hole Green's function corrected to first order by a proper self-energy is obtained [Fig. 1(c)]. Its energy trace is the desired correction to the free-hole density. The thermodynamic potential in Fig. 1(b) is a sum over contributions from pair states with different linear and angular momentum K and L. By taking the derivative of only those terms in Ω with $L=K=0$, we can select the density of the optically active holes:

$$\pi l^2\rho_h^{\rm act}=\sum_n \left[f_h(n)+\frac{1}{\beta}\sum_{i\hbar\omega_h}[i\hbar\omega_h-E_h(n)+\mu_h]^{-2} \times\Sigma_h^{\rm act}(n;i\hbar\omega_h)\right] . \tag{15}$$

$\Sigma_h^{\rm act}$ is a proper self-energy,

$$\Sigma_h^{\rm act}(n;i\hbar\omega_h)=\frac{1}{\beta}\sum_{i\hbar\omega_e} G_e(n,i\hbar\omega_e) \times K(n,n;i\hbar\omega_e+i\hbar\omega_h) , \tag{16}$$

where the electron Green's function (in the quasiparticle approximation)

$$G_e(n,i\hbar\omega_e)=[i\hbar\omega_e-E_e(n)+\mu_e]^{-1} \tag{17}$$

and the scattering matrix

$$K(n,m;i\hbar\omega)=\sum_i \frac{\Psi_i(n)^*\Psi_i(m)}{i\hbar\omega-\lambda_i}{\rm sgn}(\lambda_i-\mu_e-\mu_h) - V_{eh}^S(n,m) , \tag{18}$$

$$\Psi_i(n)=\sum_{n'} V_{nn'}^S\sqrt{|F(n')|}\phi_i(n') \tag{19}$$

have been introduced. Similar expressions for the self-energy of a positron in a metal have been derived by Arponen.[19] When the number of holes is sufficiently small the electron chemical potential will not be affected and the holes may be treated classically by $\beta\mu_h\to-\infty$. Using Eqs. (16)–(19) the limiting value of Eq. (15) becomes after few manipulations

$$\lim_{\beta\mu_h\to-\infty}\pi l^2\rho_h^{\rm act}=\sum_n(e^{-\beta[E_h(n)-\mu_h]}-e^{-\beta[E(n)-\mu_e-\mu_h]}) +\sum_i e^{-\beta(\lambda_i-\mu_e-\mu_h)} , \tag{20}$$

which is the central result of this section.[23,24] If $\lambda_{\rm ex}$ is used to denote the lowest eigenvalue which does not equal any $E(n)$, the hole in the ground state behaves like a free particle when $\lambda_{\rm ex}-\mu_e<E_h(0)$, and is bound otherwise, for any static interaction potential. At zero temperature and magnetic field (disregarding the state dependence of the self-energy) the exciton is thus occupied when its binding energy relative to the Fermi edge exceeds $\hbar^2k_F^2/2m_h$, where k_F is the Fermi wave vector. For a discussion of the consequences for the photoluminescence spectra, it is convenient to classify the solutions of Eq. (3) as excitonic states (index α) and free pair states (index γ), which are defined by the conditions $\forall n\Longrightarrow\lambda_\alpha\neq E(n)$ and $\exists n_\gamma\Longrightarrow\lambda_\gamma=E(n_\gamma)$, respectively. The free pair states only exist at temperatures $1/\beta\ll\mu_e$. In this case only the first term on the right-hand side contributes in Eq. (20). By taking carefully the low-temperature limit of Eq. (14) one obtains for the luminescence oscillator strengths of the free pair states with index γ,

$$F^{\rm lum}(\hbar\omega)=\sum_\gamma\frac{\delta(\hbar\omega-\lambda_\gamma)}{\pi l^2}\frac{e^{-\beta E_n(n_\gamma)}}{\sum_n e^{-\beta E_n(n')}} \times\left|1+\sum_\alpha\frac{\Psi_\alpha(n_\gamma)^*\sum_m\phi_\alpha(m)\sqrt{F(m)}}{\lambda_\alpha-\lambda_\gamma}\right|^2 . \tag{21}$$

The squared expression is an excitonic enhancement factor of the luminescence,[11] which has an equivalent in the enhancement factor of the positron annihilation rate in high-density metals.[18] The enhancement factor seems to be singular since with vanishing field $\lambda_\alpha-\lambda_\gamma$ may become infinitesimally small. In positron physics this has often been interpreted as a breakdown of the ladder approximation in the low-density limit.[21] However, closer inspection of the expression Eq. (21) reveals that it is well behaved. Furthermore, if a bound state becomes occupied, Eq. (21) is not applicable anymore. One should return to Eq. (14), in which after substituting Eqs. (12) and (20) the hole chemical potential can be divided out, and the limiting procedure does not cause any problems. So there is a discontinuity, but no divergence, in the luminescence, which is due to a change of the nature of the ground state.

IV. COMPUTATIONAL RESULTS

In numerical calculations the number of Landau-level pair states in Eqs. (3) and (4) is finite and the convergence of the expansion must be carefully monitored, especially in the limit of small magnetic fields. At 0.2 T a basis set of $\simeq$600 Landau levels is necessary for accurate results, a number which decreases rapidly for higher magnetic fields. It has been checked explicitly that the additional approximation of replacing the Coulomb matrix elements in the self-energies V_{ee} and V_{hh} by V_{eh} does not introduce significant errors. The parameters for GaAs $m_e=0.067$, $m_h=0.3$, $\kappa=12.5$ for well and barrier material and a valence-band–conduction-band offset ratio of 0.3/0.7 are used. All results are for a 100-Å GaAs/$Al_{0.3}Ga_{0.7}As$ quantum well, since results for other growth parameters

(in the range of the validity of the present model) have been found qualitatively the same. Very low densities have been discussed in Refs. 7 and 22 in Hartree-Fock theory, and it remains to be investigated whether the present approximation scheme is a meaningful improvement in that regime. At very high densities, on the other hand, the excitonic effects appear to be already quite well understood. Therefore results are presented here for the intermediate density regime only, although arbitrary densities can be handled by the programs.

A. Zero magnetic field

The luminescence spectra of a 100-Å quantum well are plotted in Figs. 2–4 as a function of density and temperature in the regime where the transition from bound to free hole occurs. Figure 2 clearly illustrates the counterintuitive result that the photoluminescence at very low temperatures can be dominated by the exciton, even when the actual band gap is smaller than the exciton energy.[23,24] A discontinuous (at zero temperature) appearance of a Stokes shift between absorption and luminescence is found at a critical density $\rho_c \simeq 10^{11}$ cm^{-2}. The sudden redshift of the luminescence reflects the transition from exciton to free-particle-like behavior discussed above. At a slightly higher temperature (Fig. 3) two peaks appear, one from the recombination of the ground state and one from the excited state, which is a consequence of thermal population as well as the thermally induced Coulombic matrix elements between these states. The ground and excited states are bound and free, respectively, at densities lower than ρ_c, vice versa for densities higher than ρ_c. At helium temperature (Fig. 4) the transition density region is increased and the two peaks are much less pronounced. At even higher temperatures it does not make sense anymore to talk about an unbinding transition at all. The absorption spectra (not shown) do not display any such discontinuity. The exciton binding energy relative to the absorption edge and the exciton oscillator strength decreases with increasing density,[24] in accordance with earlier studies.[7]

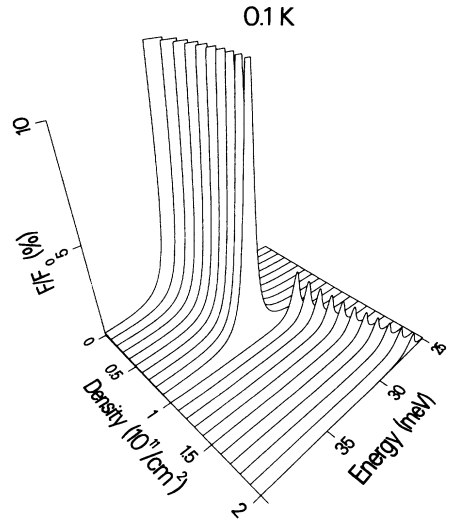

FIG. 2. Perspective view of the calculated photoluminescence oscillator strengths F as defined in Sec. III for a 100-Å GaAs/$Al_{0.3}Ga_{0.7}As$ symmetrically modulation-doped quantum well at 0.1 K. F [Eq. (14)] is expressed in percent of the oscillator strength of the strictly 2D ground-state exciton $F_0 = 16/(\pi a_B^2)$, where a_B is the exciton Bohr radius. A Lorentzian broadening parameter $\delta = 0.45$ meV has been introduced.

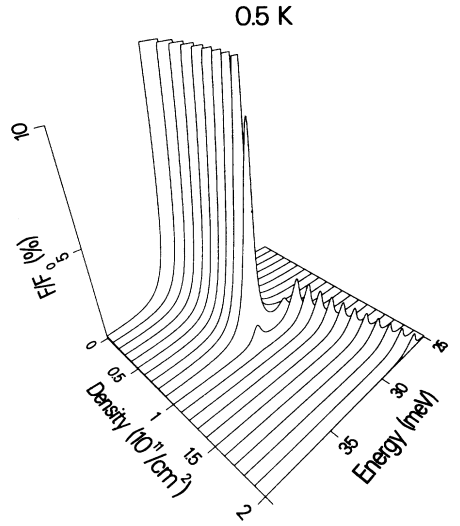

FIG. 3. As Fig. 1, but for a temperature of 0.5 K.

B. Magnetic-field effects

For a density slightly above the exciton unbinding discussed above, the magnetic-field and filling factor $\nu = 2\pi l^2 \rho_e$ dependence of absorption and luminescence spectra is plotted in Figs. 5 and 6. The zero-field broadening parameter Γ_e, which moderates the singular screening, has been chosen rather arbitrarily to be 0.1 meV, corresponding to a high-mobility sample. The re-

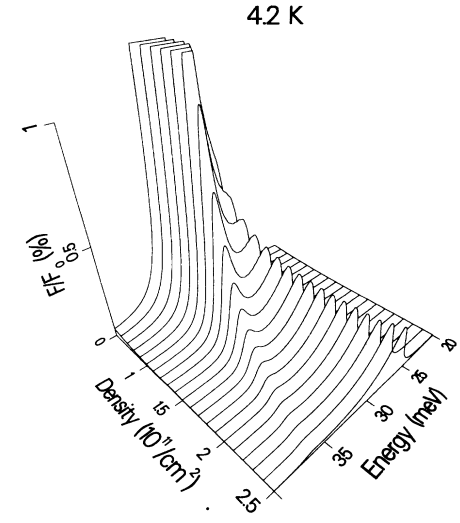

FIG. 4. As Fig. 1, but for a temperature of 4.2 K.

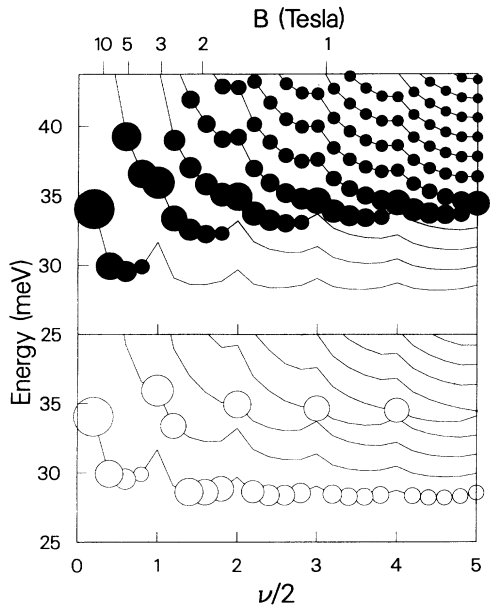

FIG. 5. Magnetoabsorption (full dots) and luminescence (open circles) spectra of a 100-Å quantum well with a density of 1.5×10^{11} cm^{-2} at 0.1 K as a function of filling factor ν. The oscillator strengths are proportional to the dot size. Due to the neglect of spin splittings, the Landau levels are completely filled at even filling factors. The self-energies are calculated in the quasistatic approximation.

sults are seen to be quite different from those in Ref. 24, where the magnetic-field dependence of the screening was not taken into account. The upward cusps of the single-particle Landau-level transitions are due mainly to the hole self-energy, which becomes less negative when the screening is reduced at even filling factors, as has been discussed in detail in Refs. 13 and 14. But the luminescence does not follow the band gap.[25] At even filling factors the increased Coulomb attraction stabilizes the excitonic ground state, which decays by emitting light which is blueshifted relative to the band gap by the electron Fermi energy. The density of states at the Fermi energy becomes large even for small deviations from completely filled levels. The Coulomb interaction is strongly screened and the exciton effectively quenched. Consequently recombination from the band gap involving the free hole takes over. The results for the same parameters, but in the plasmon-pole approximation to the self-energies, are presented in Fig. 6. The state dependence of the self-energy is larger and the total renormalization smaller than in the quasistatic approximation, but qualitatively the same effects are seen. It is concluded that at not too high magnetic fields the quasistatic approximation does not introduce gross errors in spite of its simplicity.

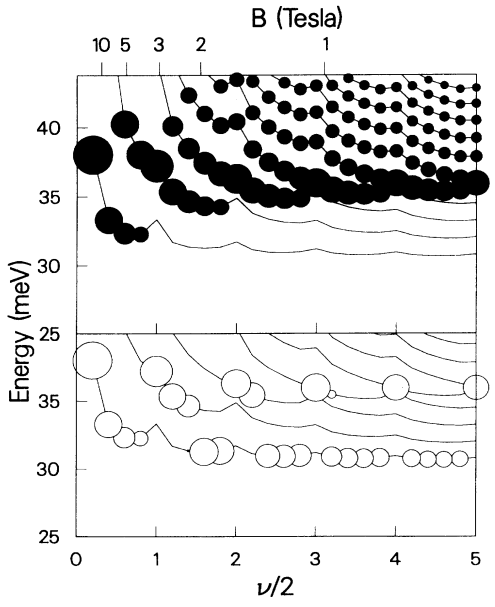

FIG. 6. As Fig. 5, but self-energies are calculated in the plasmon-pole approximation.

V. LIMITS OF THE PRESENT THEORY

A faithful model for the quantum-well structure and the nonlocal and magnetic-field-dependent screened interaction render an exact calculation of the optical spectra impossible. The question thus arises if the predictions of the mean-field approximation can be trusted. In the following, several complications are discussed which could invalidate mean-field theory in its present form.

A. Lifetime broadening and screening

The imaginary part of the single-particle self-energies, i.e., the lifetime broadening due to many-body effects, has been disregarded here.[28,34] Impurity scattering also broadens the energy levels, and has been taken into account only by its effects on the screening. The total broadening has been treated here simply by replacing δ in Eq. (1) by a phenomenological parameter. Extremely narrow linewidths have been observed in doped systems with very high mobilities.[35–38] Since impurity scattering is very small in these systems, it may be concluded that the broadening due to many-body processes also can be very small.

Dynamical screening complicates the Bethe-Salpeter equation enormously,[28] and its effects are very difficult to assess in all generality. In Ref. 28 a phenomenological reduction of the static screening has been introduced to model dynamical screening, which would increase excitonic effects even more than reported here. Dynamical screening has been found to cause effects in highly excited quantum wells,[27,39] but the problem of the static screening approximation appears to be associated mainly with the contribution from the hole plasma, which is of no concern here.

The above calculations may also exaggerate the modulation of the screening. The unavoidable density of states between the Landau levels is neglected in the self-consistent Born approximation, and the quenching of the screening at even filling factors is possibly less efficient

than assumed here. The reentrant exciton binding phenomenon will then occur only at somewhat lower densities than calculated here. If the broadening is of the order of the Landau-level spacing, the zero-field screening function as used in Ref. 24 is more appropriate.

B. Excitonic corrections to hole self-energy

A concern at lower densities is the nature of the hole propagator and the applicability of the quasiparticle approximation for the hole. A better approximation of the hole structure is provided by summing the proper self-energies, which have been taken into account in Fig. 1(c) only to first order.[19] The effect of the finite exciton mass is small and vanishes for infinite hole mass. If the exciton dispersion is neglected, the excitonic correction is easilly calculated using the solutions of the Bethe-Salpeter equation,

$$\Sigma_h^{\rm exc}(i\hbar\omega_h)\simeq-\sum_{\alpha,n}\frac{2|\Psi_\alpha(n)|^2 f_e(n)}{i\hbar\omega_h-\lambda_\alpha+E_e(n)}\ . \tag{22}$$

The poles of the hole Green's function $\lambda_p(n)$ are solutions of Dyson's equation,

$$\lambda_p(n)-E_h(n)=\Sigma_h^{\rm exc}(\lambda_p(n))\ . \tag{23}$$

In terms of the renormalization factors

$$Z_p(n)=\left[1-\frac{\partial\Sigma_h^{\rm exc}(\lambda)}{\partial\lambda}\right]^{-1}\Bigg|_{\lambda=\lambda_p(n)}, \tag{24}$$

the spectral function of the holes becomes

$$A_h(n,E)\simeq\sum_p Z_p(n)\delta(E-\lambda_p(n))\ . \tag{25}$$

A possible improvement of the present mean-field treatment of the optical spectra is the replacement of the free-hole propagator in the electron-hole Green's function by the renormalized one. Though this program is not carried out here, an impression of the importance of such a correction is given by the hole spectral function $A_h(0,E+E_h(0))$ which is plotted in Fig. 7 as a function of density. At very high and very low electron densities the exciton effect is small, but at intermediate densities the situation is more complicated. At 2×10^{11} cm^{-2} the exciton coupling causes a weak high-energy tail to the quasihole peak, and a small excitonic contribution to the band-gap renormalization is also observed. With decreasing density a sharp peak develops at the high-energy edge of the tail, which finally takes over all spectral strength. The results may be interpreted as a mixing of the free and bound ground states, which did not have matrix elements in the mean-field approximation. This explicitly demonstrates how the abrupt transition is smeared out by higher scattering processes. Still a full renormalization will not change the mean-field results drastically. At the critical density of 10^{11} cm^{-2} the weight of the high-energy feature is only $Z=0.2$, and the jump in the luminescence should survive a full renormalization. Only at lower densities do we have a well-resolved doublet structure, which might cause observable effects in the optical spectra. A small effective temperature is expected to cause very similar effects. It is rather striking that, in spite of the conclusion that a relatively abrupt unbinding should remain observable, the spectral function of the hole changes smoothly with density. The reasons are continuity of the hole Green's function even at the mean-field level, and the difference in the way that the ladders enter the diagrams for one- and two-particle properties.

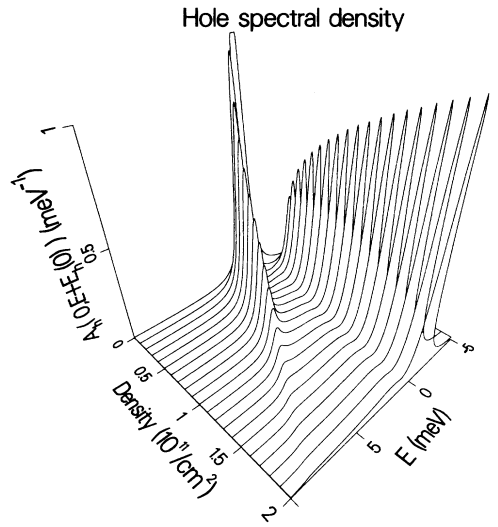

FIG. 7. Spectral density of the hole single-particle Green's function as modified by the coupling to the excitonic bound state [see Eqs. (22)–(25)].

C. Other higher-order scattering processes

Another set of higher-order scattering diagrams are the corrections to the ladder approximation of the vertex corrections. Typical representatives of these are diagrams in which the Coulomb interaction lines cross. These vanish unless the Fermi sea has been "shaken up" by the perturbing potential of the hole to create empty states below the Fermi energy. When the electron-hole interaction strength is sufficiently small, only the states close to the Fermi edge are affected. Consequently one would expect significant contributions from these diagrams at energies close to the absorption edge. Outside this narrow spectral region, crossed and other diagrams are unlikely to be important. So the conclusion is that, close to the unbinding transition, the corrections should be small, but might become important at lower densities.

The higher-order electron-hole scattering terms in a perturbative treatment can be summed exactly when the electron-hole interaction is represented by a separable or contact interaction, and for an infinitely massive (core) hole.[4] For such a simplified model it is therefore possible to test the accuracy of the mean-field (ladder) approximation directly. Ohtaka and Tanabe found the ladder approximation to represent exact results faithfully when the interaction strength is small compared to the Fermi energy. According to the criterion derived above, the binding energy at ρ_c is only a fraction m_e/m_h of the Fermi ener-

gy, which means that the ladder approximation is expected to be applicable. This conclusion was confirmed by the good agreement of mean-field spectra[25] with those calculated by Uenoyama and Sham.[16] Unfortunately the regime where bound states become important was not covered.

Hawrylak[17] went further than Uenoyama and Sham[16] by including a realistic Coulomb potential and considering bound-state effects. His result that the Fermi-edge singularity is washed out by a finite hole mass is difficult to understand and not compatible with the present ones for the following reasons. For the infinite hole mass it is well established that the δ-function singularity of the bound excitonic state is weakened by higher-order processes into a power-law behavior. Still, for the infinite hole mass, there is evidence that the bound state significantly affects the optical spectra, and only the details of the line shape are modified by a treatment beyond mean-field theory.[4,16] When the finite mass of the hole is taken into account, the binding energy and oscillator strength of the bound state decrease, but are still very significant as shown above. Higher-order scattering processes reflect the response of the electron gas to the perturbing hole, which is most important for a massive hole and vanishes with vanishing hole mass. Consequently, the accuracy of mean-field theory should improve with decreasing mass of the hole, and the infinite hole mass is the most stringent test case. In other words, a bound state found in mean-field theory should remain increasingly intact when the hole mass decreases. These conclusions are not reflected by Hawrylak's results.[17] The effects of the additional approximations introduced in Ref. 17 to treat the hole recoil are difficult to estimate and might be responsible for this conundrum.

D. Optically inactive bound states and nonequilibrium

It should be kept in mind that we have derived only the oscillator strength of the luminescence in thermal equilibrium. In actual experiments hole relaxation dynamics might be important, causing nonequilibrium effects beyond the present formalism, e.g., different electron and hole temperatures. Experimental luminescence spectra should also be divided by the density of optically active holes to be comparable with the present results, and the latter might be difficult to estimate. A complication might arise from the bound states with finite translational or rotational momentum, which at higher doping densities can have a lower energy than the optically active s-type excitons at rest. This effect is rather subtle at zero magnetic fields, but becomes very obvious in high magnetic fields. Take, e.g., one Landau level ($n=0$) to be completely occupied. The optically active spherically symmetric (s-type) exciton state is then associated with the transition between the second Landau levels ($n=1$), but the optically forbidden (p^+-type) exciton associated to the transition from the first hole to the second electron Landau level has clearly a lower energy. When the temperature is sufficiently high so that allowed states are occupied and decay channels exist which prevent accumulation of a high hole density in the forbidden states, the present results are applicable. If, on the other hand, the holes are in thermal equilibrium at very low temperatures, the luminescence initially will be zero. The holes then accumulate until states become occupied which are allowed to decay. "Nonlinear" effects due to the additional hole gas could thus be significant.

VI. COMPARISON WITH EXPERIMENTS

At this moment there is no unambiguous experimental evidence for the exciton (un)binding transition. However, it should be stressed that most previous optical experiments on modulation-doped quantum wells have been carried out at high doping densities and temperatures. Furthermore, the sample quality is generally not sufficient, since a luminescence linewidth of typically 5 meV would render the subtle many-body effects unobservable. From Figs. 2–4 we saw that a carrier temperature of $\lesssim 1$ K and a luminescence linewidth of $\lesssim 1$ meV are required. These conditions are met only by recent experiments on high-mobility samples.[35–38] Especially for the experiments on high-mobility heterojunctions, temperature and sample quality should not cause any problems, but unfortunately the complicated structure of spatially separated electrons and holes and a second electronic confinement state close to the Fermi energy makes a direct comparison difficult. On the other hand, most experimental features are well described by a reentrant exciton (un)binding transition, where the excitonic state is associated to the second electron subband,[25] while a theory[40] which takes the second subband into account explicitly cannot explain the experiments on these high-quality samples. Since the spin splitting of the electron states is larger than the Landau-level broadening, the exciton binding is observed at even as well as odd filling factors.[36] The recently resolved quenching of the lower-energy luminescence line at integer filling factors[37] is important evidence in support of the exciton unbinding model. In experiments on narrower quantum wells[38] the present two-band model should be applicable. The present theory cannot make any statements about the observed modifications of the free-hole luminescence in these samples at filling factor unity. A search for an exciton unbinding transition should be concentrated on filling factors $\nu \leq 2$ and even smaller densities than considered in Ref. 38.

VII. CONCLUSIONS

In summary, the following picture for the optical properties of modulation-doped quantum wells emerges. The absorption spectrum changes undramatically when the quantum well is increasingly filled by electrons. The Wannier exciton at zero density develops continuously into the Mahan exciton (or Fermi-edge singularity) at high densities. On the other hand the luminescence spectra are affected by a transition from a bound to a free ground state, which is predicted to occur at densities of $\simeq 10^{11}$ cm^{-2}. The abruptness of the transition is destroyed by finite temperatures and higher-order scattering processes, but is believed to remain observable in the luminescence spectra of high-quality samples at

sufficiently low temperatures. An unambiguous sign of the transition is a doublet structure with an energy separation of the electron Fermi energy. An oscillatory behavior in the magnetoluminescence with abrupt blueshifts at even filling factors would be strong evidence of the (un)binding transition, which can be reentrant with increasing magnetic field.

In mean-field theory the (un)binding transition should occur in any dimension. It is quite possible though that the conditions for an observability are best for quasi-2D systems. Due to the increase of the exciton binding energy in quasi-2D, the exciton remains stable in mean-field theory up to such high densities that higher-order scattering processes cannot cause much harm anymore. In three-dimensional systems the transition density is probably too low to allow clear effects to be observed. Quasi-one-dimensional confinement, on the other hand, increases the exciton effect even more, and it may be found that the transition density cannot be reached in quantum wires by conventional modulation doping, which would mean that the unbinding might again not be observable.

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APPENDIX

In the main text the advantages of solving the Bethe-Salpeter equations by applying a small magnetic field have been emphasized. The drawback is a large number of Coulomb matrix elements, which involve integrals such as Eq. (7). For small quantum numbers these are easily obtained analytically by insertion of the Laguerre polynomials. At low magnetic fields, however, several hundred Landau levels have to be included into the basis to obtain converged results. As noted by Chu and Chang,[41] a floating point summation of the expressions obtained by a power expansion will break down because of the rounding errors caused by very large positive and negative terms. The same authors proposed an alternative double summation of positive coefficients for the matrix elements of the bare potential, which can be evaluated accurately. Unfortunately, this approach appears to become prohibitively time consuming when screening is included. On the other hand, with increasing quantum numbers it becomes attractive to use semiclassical approximations, where strongly oscillating terms are averaged out. In the present study Titeica's[42] semiclassical approximation of the generalized Fourier transform J_{mn} has been found very useful:

$$J_{mn}(q)^2=\frac{1}{\pi}[(m+n+1)q^2l^2-(m-n)^2-q^4l^4/4]^{-1/2} \tag{A1}$$

for $q\in\{q_1,q_2\}$, where

$$q_{1,2}^2l^2=2[(m+n+1)\pm\sqrt{(2m+1)(2n+1)}] \tag{A2}$$

and zero otherwise. A complication is the divergence of the integrand in Eq. (7) when Eq. (A1) is employed for $m=n$ and the bare Coulomb potential, or at integer filling factors where the polarizabilities vanish for vanishing wave vector. In that case a small q expansion of the integrand in Eq. (7) should be integrated up to a cutoff of the order of $q_cl=1/\sqrt{2m}$, which then replaces q_1 as the lower integration limit in the semiclassical expression. The accuracy of the semiclassical approximation for the matrix elements is worst for the diagonal elements, which are compared with the exact results in Fig. 8. We see that the agreement is astonishingly good even for $m=1$. Due to the rapid variation of the polarization function close to $q=0$ at large integer filling factors, the approximation for the diagonal elements becomes less accurate. But although the diagonal elements might be off by 20% in these unusual cases, the effects on the spectra are still hardly observable.

Other advantages of the expression Eq. (A1) is the possibility to evaluate infinite summations over the Landau-level indices, as occurring, e.g., in the calculation of polarizabilities in the presence of magnetic fields. The virtual excitations from an occupied Landau levels with index m to all empty Landau levels with indices larger than N_c (Ref. 12) is approximated by the simple expression

$$\sum_{n=N_c}^{\infty}\frac{J_{nm}(q)^2}{n-m}\simeq\frac{1}{lq}\frac{1}{\sqrt{l^2q^2/4-2m-1}} \tag{A3}$$

for those values of q which render the square root real. It is also easy to correct for basis-set limitations by Löwdin perturbation theory.[43] The calculations of the dynamic Stark effect for strictly 2D systems reported in Ref. 22

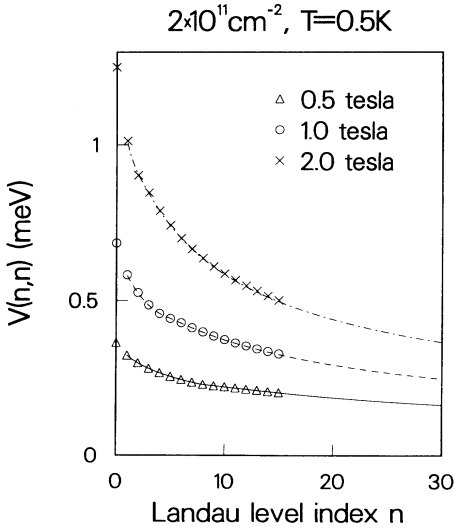

FIG. 8. Diagonal elements of the screened Coulomb interaction matrix Eq. (7) at a density of 2×10^{11} cm^{-2}, a temperature of 0.5 K, and different magnetic fields. The results obtained by summing the series obtained by inserting the Laguerre polynomials (markers) are compared with the semiclassical approximation (continuous lines).

are practically converged for small fields with a basis of 1200 Landau levels, while Stafford, Schmitt-Rink, and Schäfer[44] report lack of convergence even for a basis of 1700 Landau levels and high magnetic fields. It should also be mentioned that the presence of the form factor improves convergence dramatically, and a few hundred Landau levels are in general sufficient for fields above 0.2 T.

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