Line shapes of intersubband and excitonic recombination in quantum wells: Influence of final-state interaction, statistical broadening, and momentum conservation

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A realistic and comprehensive theory of line shapes for spontaneous recombination of twodimensional carriers in quantum-well (QW) structures is developed. Starting from the line shape for intersubband recombination, which takes into account the QW density of states and the thermal carrier distribution function, the impact of momentum (non)conservation on the luminescence line shape is considered. Then Lorentzian broadening due to the finite lifetime of the final states and Gaussian broadening due to statistical fluctuations of quantum-well eigenenergies characteristic, e.g., of interface roughness is incorporated. The effects of Coulomb interaction of the charge carriers at low densities are considered quantitatively, including both excitonic bound states and excitonic enhancement above the two-dimensional band gap. For a case study, GaAs QW luminescence line shapes are investigated. The line-shape evaluation definitely proves that recombination is excitonic at any temperature up to 300 K in contradiction to previous assumptions of some other authors. At low temperatures all lines consist, on a first view, of unresolved doublets which are very close in energy. The high-energy component is identified as the free-electron-heavy-hole exciton. Momentum is not found and does not need to be conserved in the free-exciton recombination process at low temperatures. At high temperatures, momentum conservation is found to be reestablished: Momentum conservation is understood to depend on the relative amplitude of interfaceroughness-induced lateral potential fluctuations as compared to the thermal energy of the excitons.

I. INTRODUCTION

The objective of this paper is twofold. (1) First of all a comprehensive and realistic theory of luminescence line shapes of quantum wells (QW's) is presented. It has been recognized that a deconvolution of experimental OW line shapes might provide quantitative, otherwise inaccessible information on structural and chemical properties of the two interfaces of the QW (Refs. 1 and 2) or on impurity incorporation^{3,4} at the growth surface as a function of growth parameters. Excitons (or electron-hole pairs) are ideal sensors of atomic scale chemical and structural properties of layers only a few atoms thick as well as of their interfaces to adjacent layers of different chemical composition. They act similar to the tip of a scanning tunnel microscope (STM),⁵ yielding, however, information on regions not accessible to STM's far below the surface with a principal lateral measure given by the twodimensional exciton diameter of $d_X \approx 20$ nm. Characterization and controlled modification of interfaces are crucial to all advanced microstructured photonic and electronic devices. In view of such applications a line-shape theory has to distinguish and treat separately the cases of free-electron-free-hole recombination and excitonic recombination for the cases of conservation and nonconservation of the wave vector. Additionally recombination lines are broadened due to the thermal distribution of the carriers,^{1,6} due to statistical effects caused by interface roughness^{7,8} or composition fluctuations, 9^{-11} and due to final-state interaction^{8,12} causing Lorentzian broadening. Ab initio neglection of any of these effects without physical justification leads to invalid or inconclusive results. Parts of such a line-shape theory were established by $us^{1,6,8}$ and others^{13,14} recently. But some of the previous results are unfortunately qualitatively incorrect^{13,14} (e.g., the role of wave-vector conservation was incorrectly treated¹⁴). Our own preliminary work^{1,6,8} already incorporated all essential broadening mechanisms mentioned above, however, excitonic and *e*-*h* recombination with and without **k** conservation were not separately treated.

(2) We will not restrict ourselves here to the presentation of the details of the line-shape theory but we will demonstrate the value and power of such detailed treatment by applying it to some experimental results obtianed by us, in order to resolve two long lasting disputes on (a) whether, and under which circumstances, the *wave vector is conserved* in recombination in QW's and (b) whether the room-temperature (RT) recombination at least in the well-known GaAs model system is predominantly *excitonic or free-electron-free-hole* in nature.

Various authors (e.g., Ref. 13) have suggested that for low excitation at *room temperature* the spontaneous emission from undoped GaAs QW's may not obey \mathbf{k} conservation. Our results prove that it does. At very low temperatures, however, \mathbf{k} does not need to be conserved since the carriers (excitons) are spatially localized in potential fluctuations caused, e.g., by interface roughness.

Other authors¹⁵ have recently concluded that the origin of room-temperature luminescence in GaAs QW's is free-electron-free-hole recombination in contrast to earlier suggestions by us^{16,17} and others.¹⁸ We will show here that the origin is unambiguously excitonic in single QW's in high-quality material. In strongly coupled QW's or superlattices the situation is different.^{19,20}

The paper is organized as follows. In Sec. II line shapes for interband recombination in an idealized quantum well are presented for momentum and nonmomentum conservation. Lifetime broadening and statistical broadening are successively introduced in Secs. III and IV. Excitonic line shapes are presented and discussed in Sec. V. In Sec. VI the theory is applied to experimental GaAs QW spectra at 2 and 300 K in order to resolve the above-mentioned disputes.

II. FREE-ELECTRON-HOLE-RECOMBINATION LINE SHAPES

The spontaneous emission rate $R(h\nu)dh\nu$, i.e., the number of photons which are emitted per second within an energy interval $[h\nu, h\nu+d h\nu]$ for interband recombination in an optically isotropic medium is given by Fermi's golden rule^{21,22} and considering only one valence (VB) and one conduction band (CB)

$$R(h\nu)dh\nu = \sum_{\mathbf{k}_{c},\mathbf{k}_{v}} \frac{4ne^{2}h\nu}{m^{3}\hbar^{3}c^{3}} |M|^{2}f_{c}(1-f_{v})\delta(E_{c}-E_{v}-h\nu) ,$$
(1)

 f_c and f_v are the occupation probabilities of the upper and lower states of the transition, respectively, *n* is the index of refraction, and the matrix element *M* is averaged over all polarizations of light. Converting the summations in Eq. (1) into integrals over the corresponding wave vectors \mathbf{k}_c and \mathbf{k}_v , we have to distinguish between two cases: \mathbf{k} conservation and *non*- \mathbf{k} conservation.

In the former case the matrix element will contain an additional δ function $\delta(\mathbf{k}_c - \mathbf{k}_v - \mathbf{k}_j)$ which equals $\delta(\mathbf{k}_c - \mathbf{k}_v)$ if we neglect \mathbf{k}_j (**k** vector of the photon) which is typically much smaller than \mathbf{k}_c and \mathbf{k}_v . If we further neglect any explicit **k** dependence of the dipole matrix element we obtain

$$R(h\nu) \sim \int_{c} d\mathbf{k}_{c} \int_{v} d\mathbf{k}_{v} f_{c} (1-f_{v}) \\ \times \delta(E_{c}-E_{v}-h\nu) \delta(\mathbf{k}_{c}-\mathbf{k}_{v}) . \quad (2)$$

The last term on the right-hand side holds for \mathbf{k} conservation. After converting the integration over \mathbf{k} into an integration over energy we obtain, providing non- \mathbf{k} conservation

$$R(h\nu) \sim \int_0^\infty dE_c \int_0^\infty dE_v \rho_c(E_c) \rho_v(E_v) f_c(E_c) \times [1 - f_v(E_v)] \delta(E_c - E_v - h\nu) .$$
(3a)

For the case of \mathbf{k} conservation we obtain,

$$R(h\nu) \sim \int_0^\infty dE_c \rho_{\rm red}(E_c - E_v) f_c(E_c) [1 - f_v(E_v)] \\ \times \delta(E_c - E_v - h\nu) , \qquad (3b)$$

where ρ_c , ρ_v , and ρ_{red} are the conduction-band, valenceband, and the reduced density of states, respectively, and f(E) is the occupation probability of a state with energy E.

Let us now consider a semiconductor with isotropic and parabolic dispersion of energy in the (x,y) plane as,

$$E_{c}(\mathbf{k}_{c}) = \frac{\hbar^{2}}{2m_{e}}k_{c}^{2} + E_{g}(L_{z}) , \qquad (4a)$$

$$E_v(\mathbf{k}_v) = -\frac{\hbar^2}{2m_h} k_v^2 , \qquad (4b)$$

where E_g is the L_z -dependent two-dimensional (2D) band gap. Inserting the step function $\Theta(E)$ for the density of states we eventually get for the case of non-**k** conservation,

$$R(h\nu) \sim \int_0^\infty dE_c \int_{-\infty}^0 dE_v m_e m_h f(E_c) \times [1 - f(E_v)] \delta(E_c - E_v - h\nu)$$
(5a)

and for k conservation

$$R(h\nu) \sim \int_{0}^{\infty} dE_{c} \frac{m_{e}m_{h}}{m_{e}+m_{h}} \Theta([(m_{e}+m_{h})/m_{h}](E_{c}-E_{g}))f(E_{c})[1-f((m_{e}/m_{h})(E_{g}-E_{c}))] \times \delta([(m_{e}+m_{h})/m_{h}]E_{c}-(m_{e}/m_{h})E_{g}-h\nu) ,$$
(5b)

$$R(h\nu) \sim \frac{m_e m_h}{m_e + m_h} \Theta(h\nu - E_g) f(\varepsilon_c + E_g) [1 - f(-\varepsilon_v)], \qquad (5c)$$

 $\varepsilon_{e(h)}$ are the reduced conduction- and valence-band energies, respectively:

$$\varepsilon_{e(h)} = \frac{m_{h(l)}}{m_e + m_h} [h v - E_g(L_z)].$$
 (5d)

In the limiting case of Boltzmann statistics Eq. (5c) simplifies to

$$R(h\nu) \sim \frac{m_e m_h}{m_e + m_h} \Theta(h\nu - E_g) \exp[-(h\nu - E_g)/kT_c)] .$$
(6a)

The half-width [full width at half maximum (FWHM)] of the recombination line is thus proportional to the carrier temperature T_c

$$FWHM = kT_c \ln 2$$
.

(6b)

Equation (5a), which is valid only for recombination without conservation of **k**, corresponds to Eq. (1) of Ref. 14, although these authors claim that momentum conservation is a prerequisite for its derivation. From Eq. (5c) we learn, that in the case of **k** conservation, *R* is *not* given by a convolution of the valence- and conduction-band density of states with their respective occupation probabilities but simply by a *product* of the *joined density of states* and the occupation functions $f_c(1-f_v)$.

III. LIFETIME BROADENING

The recombination of an electron in the CB with a hole in the VB leaves a hole in the (thermal) electron distribution function of the CB and vice versa. The distribution function will be reestablished by a rearrangement of the carriers within a certain scattering time, resulting in a finite lifetime $\tau(E_{e})$ (h) of the final state of the recombination process. We will now describe this final-state interaction using a model analogous to that first established by Landsberg for the emission spectra of x rays two decades ago.^{23,24} Each discrete energy level in Eq. (5b) has to be replaced by a Lorentzian broadened level, with a broadening parameter $\Gamma = h/\tau$. Thus the probability P per unit energy range of finding a carrier at energy E_c due to the broadening of a level at the energy E'_c of halfwidth $\Gamma(E'_c)$ is,

$$P(E_{c}, E_{c}') = \frac{1}{2\pi} \frac{\Gamma(E_{c}')f(E_{c}')\rho(E_{c}')}{(E_{c} - E_{c}')^{2} + \frac{1}{4}\Gamma^{2}(E_{c}')} , \qquad (7a)$$

$$P(E_{c}, E_{c}') = L(E_{c}, E_{c}')f(E_{c}')\rho(E_{c}') , \qquad (7b)$$

where L is the Lorentz function. In order to obtain the contributions of all broadened states at energies E'_c to the energy E_c we have to integrate over all E'_c 's. This broadening mechanism acts on electrons *and* holes. Consequently, we have to replace Eq. (5b) by

$$R(h\nu) \sim \int_0^\infty \Theta(E' - E_g) f(\varepsilon_c') [1 - f(\varepsilon_v')] L(h\nu, E') dE'.$$
(8)

The broadening parameter $\Gamma(E')$ is, in general, a complicated function of E'. One has to sum up over all possible scattering processes, and even in the case of Fermi statistics at T = 0 K $[f(E') = \Theta(E_F - E')]$ the expression remains very complex.²³ Obviously the dominating contribution stemming from the final-state interaction $\Gamma(E')$ reaches a maximum at the band extrema and decreases with increasing E'. For the sake of simplicity we assume $\Gamma(E')$ to be proportional to the number of carriers having energies E'' > E':

$$\Gamma(E') = \Gamma_0 \int_{E'}^{\infty} \rho(E'') f(E'') dE'' .$$
(9)

If we assume Boltzmann statistics, Eq. (9) can be simplified and we obtain for Eq. (8)

$$R(h\nu) \sim \int_{E_g}^{\infty} \frac{\Gamma_0 \exp\left[-2\frac{E'-E_g}{kT_c}\right] dE'}{(h\nu-E')^2 + \frac{\Gamma_0^2}{4} \exp\left[-2\frac{E'-E_g}{kT_c}\right]} .$$
 (10)



FIG. 1. (a) Theoretical luminescence line shape, calculated for different lifetime broadening parameters Γ_0 according to Eq. (11). (b) Statistically broadened QW luminescence line shape [Eq. (16a)], calculated for different values of the standard deviation σ_E .

By using $\gamma = \Gamma_0 / 2kT_c$, $y = (E' - E_g)/kT_c$, and $x = (hv - E_g)/kT_c$ we obtain for the line shape

$$I(hv) \sim \gamma \int_0^\infty \frac{\exp(-2y)}{(x-y)^2 + \gamma^2 \exp(-2y)} dy \quad . \tag{11}$$

Figure 1 shows theoretical line shapes according to Eq. (11) for various values of Γ_0 . For $\Gamma_0 >> kT_c$, e.g., for large γ , the function described by Eq. (11) looks more and more like a simple Lorentzian, whereas for increasing T_c it becomes more and more asymmetric. As described later in Sec. V we will observe that at low temperatures the luminescence from QW's with close to ideally abrupt interfaces (no Gaussian broadening) is almost ideally Lorentzian. In general the lifetime broadening parameter Γ_0 is a function of temperature and may strongly increase with increasing lattice temperature.

IV. STATISTICAL BROADENING

Let us now consider the influence of a statistical distribution $P(E_g, \langle E_g \rangle)$ of the 2D band gap E_g due to interface roughness or alloy broadening, where P is a given

probability density function. Then the reduced density of states $\rho_{red}(E, \langle E_g \rangle)$ is obtained by summing over all energies E_g , weighted with $P(E_g, \langle E_g \rangle)$. If P is a continuous function

$$\rho_{\text{red}}(E, \langle E_g \rangle) = \int_0^\infty P(E_g, \langle E_g \rangle) \rho_{\text{red}}(E, E_g) dE_g \quad . \tag{12}$$

Providing $P(E_g, \langle E_g \rangle) = 0$, if $E_g < 0$ and $P(E_g, \langle E_g \rangle) = P(E_g - \langle E_g \rangle)$ (which is the only physically meaningful assumption), we can extend the integration interval in Eq. (12) to $-\infty$ and obtain

$$\tilde{\rho}_{\rm red}(E, \langle E_g \rangle) = P(E_g - \langle E_g \rangle)^* \rho_{\rm red}(E, E_g) , \qquad (13)$$

where * stands for convolution. To a good approximation, $P(E_g - \langle E_g \rangle)$ is given by a Gaussian^{25,26}

$$P(E_g - \langle E_g \rangle) = \frac{1}{\sqrt{2\pi\sigma_E}} \exp\left[-\frac{(E_g - \langle E_g \rangle)^2}{2\sigma_E^2}\right], \quad (14)$$

where σ_E is the standard deviation of the distribution function.

A microscopic interface model established by Singh and Bajaj^{25,26} correlates the standard deviation of the energy σ_E with atomic scale parameters of the interface,

$$\sigma_{E} = \left[\delta \sqrt{p(1-p)} \frac{d_{I}}{2a_{B}} \right] \frac{\delta E_{g}}{\delta L_{z}} \bigg|_{L_{z} = \langle L_{z} \rangle}, \qquad (15)$$

where d_I is the average lateral extension of interface islands of height δ , a_B is the L_z -dependent Bohr radius of the exciton,²⁷ p is the averaged coverage of the heterointerface, and $\langle L_z \rangle$ is the mean QW thickness.

The influence of alloy broadening, which can occur in ternary and quaternary materials, is analogously described by a statistical distribution function of the eigenenergies $P(E_g^{\text{alloy}}, \langle E_g^{\text{alloy}} \rangle)$ with a standard deviation σ_{alloy} given by^{28,29}

$$\sigma_{\text{alloy}} = 0.327 \left[c_0 (1 - c_0) \left[\frac{r_c}{a_B} \right]^3 \right]^{1/2} \frac{\delta E_g}{\delta c} \bigg|_{c=c_0}^{c_0}.$$
 (16)

Here r_c is the cluster radius and c_0 the average alloy concentration. The distribution functions $P(E_g)$ and $P(E_g^{alloy})$ are well approximated by Gaussians. Neglecting for the moment lifetime broadening [i.e., $\rho_{red}(E, E_g) = \rho_0 \Theta(E - E_g)$] we obtain from Eq. (12)

$$\tilde{\rho}_{\rm red}(E, \langle E_g \rangle) = \frac{1}{2} \rho_0 {\rm erfc} \left[\frac{\langle E_g \rangle - E}{\sqrt{2} \sigma_E} \right]$$
(17)

and

$$I(h\nu, \langle E_g \rangle) \sim \operatorname{erfc}\left[\frac{\langle E_g \rangle - h\nu}{\sqrt{2}\sigma_E}\right] f(\varepsilon_c) [1 - f(\varepsilon_v)] .$$
(18a)

Here ε_c and ε_v are defined by Eq. (4c) and $\operatorname{erfc}(x)$ is the complementary error function.³⁰ Equation (18a) describes the situation where the carriers laterally thermalize into the regions of lowest $E_g(x,y)$. If such thermalization is not effective, we have to calculate first the unbroadened line shape $I(hv, E_g)$ and then we have to con-

volute with $P(E_g, \langle E_g \rangle)$:

$$\widetilde{I}(h\nu, \langle E_g \rangle) = I(h\nu, E_g)^* P(E_g - \langle E_g \rangle) .$$
(18b)

The peak of line (18a) is shifted to lower energy with respect to the peak of line (18b) by $\Delta E = \sigma_E^2 / kT_c$ due to carrier thermalization. Thus, the spectral maximum of luminescence is not identical to $\langle E_g \rangle$ in the case of thermalization and QW widths derived from experimental peak photon energies are incorrect.

In QW samples having large statistical broadening it is indeed justified to neglect the lifetime broadening as compared to the Gaussian broadening at low excitation densities. Providing carrier thermalization the luminescence line shape is then given by Eq. (18a). Figure 1(b) shows a number of such calculated line shapes for different values of σ_E . A clear shift of the peak to low energies with increasing σ_E is observed. With increasing $\sigma_E^2/kT_c I(hv)$ becomes more and more a simple Gaussian—the thermal broadening [Eq. (6b)] becomes neglectable as compared to σ_E .

We would like to remark, however, that even at lowest temperatures the FWHM of QW luminescence is usually by no means a simple measure of the statistical broadening, although this is believed by the large majority of authors. In order to obtain meaningful results a deconvolution of the two components of the exciton doublet (see Sec. VI), an accurate analysis of each line shape and a separation of the different contributions to the FWHM is essential. With increasing temperature the contribution of the low-energy component disappears, but since thermal broadening becomes increasingly important and the FWHM again is not a simple measure of the statistical broadening. Thus incorrect results are obtained at any temperature.

Eventually we have to combine both lifetime and statistical broadening: The line-shape function Eq. (10) has to be convoluted with the Gaussian according to Eq. (18) to get the final line shape. If large growth islands are present at the interfaces, where interisland thermalization cannot take place,³¹ we have to sum over all possible



FIG. 2. Line-shape fit (solid line) of experimental luminescence data (dots) including lifetime and statistical broadening [Eq. (17)].

 $\langle E_{g} \rangle_{i}$ of the different islands:

$$I^{*}(h\nu, \langle E_{g} \rangle) = \sum_{i=1}^{n} \widetilde{I}(h\nu, \langle E_{g} \rangle_{i})^{*} P(\langle E_{g} \rangle_{i}) .$$
(19)

If L_z shows only fluctuations by 1 monolayer at each interface we have n = 3. Figure 2 shows a fit of an experimental luminescence line according to Eq. (19). Extremely large growth islands of several μ m size were directly observed using cathodoluminescence imaging.¹ Thus we have to consider three different $\langle E_g \rangle_i$ values, i = 1-3and suppressed interisland thermalization.³² (The origin of the splitting of each $\langle E_g \rangle_i$ line into a doublet is discussed elsewhere.^{4,33}) The fitting parameters Γ , σ_E , and T_c are shown in the Fig. 2. Even in this situation of largely reduced interface roughness, a finite E_g broadening within each growth island is still observable.

V. EXCITONIC EFFECTS

Equation (19) describes the line shape for interband recombination. The luminescence is conjectured, however, on the basis of time-resolved experiments to be dominated by excitonic recombination. Thus we have to include the influence of bound and unbound hydrogenic states of the free exciton on the QW luminescence line shape. Again we have to consider the question of \mathbf{k} conservation.

If k is conserved only $K \approx 0$ excitons can recombine, where K is the center of mass k vector of the exciton in the (x,y) plane. **k** conservation together with the Coulomb interaction of the electrons and holes leaves *no* degree of freedom for the recombination energy. In analogy to Elliott's theory of excitonic recombination in three-dimensional isotropic semiconductors,³⁴ one gets for the contributions of the two-dimensional $\mathbf{K} = \mathbf{0}$ exciton states below the QW subband minimum and for the excitonic enhancement above E_g :^{35,36} (1) $hv < E_g$, bound hydrogenic eigenstates at $hv = E_n$ with

$$E_n = E_g - \frac{E_X}{(n+\frac{1}{2})^2}, \quad n = 0, 1, 2, \dots$$
 (20)

and oscillator strengths f_n

$$f_n \sim (n + \frac{1}{2})^3$$
. (21a)

(2) For $hv > E_g$, the excitonic enhancement factor f_c of the oscillator strength is

$$f_{c} = \frac{2}{1 + \exp\left[-\frac{2\pi}{X}\right]},$$
 (21b)
$$X = \left[\frac{E_{X}}{hv - E_{g}}\right]^{1/2}, \quad E_{X} = \text{exciton binding energy}.$$
 (21c)

Basically the discrete eigenstates [Eq. (20)] are again lifetime and statistically broadened. After summation over all **K** eigenstates of the free exciton, assuming Boltzmann statistics and including for the time only statistical broadening, we obtain for the line shape

$$I_{X}(hv) = \frac{I_{0}}{\sigma_{E}\sqrt{2\pi}} \sum_{n=1}^{\infty} \frac{1}{(n+\frac{1}{2})^{3}} \exp\left[\frac{\left[\left(hv - \langle E_{g} \rangle + \frac{E_{X}}{(n+\frac{1}{2})^{2}}\right)^{2}\right]}{2\sigma_{E}^{2}}\right] + \tilde{I}(hv, \langle E_{g} \rangle) \frac{2}{1 + \exp\left[-\frac{2\pi}{X}\right]}, \quad (22)$$

where $\tilde{I}(h\nu, \langle E_g \rangle)$ is given by Eq. (18b). In addition one has to sum over heavy- and light-hole (hh and lh) exciton states:

$$I_X^{\text{tot}}(h\nu, \langle E_g \rangle) = \sum_{h = \text{hh,lh}} I_X(h\nu, \langle E_g \rangle)_h .$$
(23)

Again, if long-range potential fluctuations are present in the QW (e.g., large growth islands) one has to sum up over all $\langle E_g^{QW} \rangle_i$ involved, according to Eq. (19). If **k** is not conserved, the excitonic line shape is simply obtained from Eq. (18b) by replacing the joined density of states by the center-of-mass excitonic density of states, which are identical. Parabolicity of the bands and **k** independence of the matrix elements has been assumed.

VI. APPLICATION TO EXPERIMENTAL RESULTS

Figure 3(a) shows the luminescence spectrum of a 5 nm QW measured at 300 K on a semilogarithmic scale (dots).

In addition a theoretical fit using Eqs. (22) and (23) is given. The fit is close to perfect. On this scale we find some contribution of interband recombination to the luminescence. There is clear evidence, however, that the excitonic contribution absolutely predominates by nearly 1 order of magnitude. The pronounced contribution of the $\mathbf{K}=\mathbf{0}$ exciton states is beautifully displayed. The comparison to a simple interband line shape according to Eq. (19), which is additionally depicted, demonstrates clearly that the experimental observations cannot be understood neglecting excitonic effects at room temperature.

Figure 3(b) shows low-temperature luminescence data together with a fit according to the model assuming no k conservation. Although at $T_c = 15 \text{ K} (kT_c \approx 1 \text{ meV})$ only the lowest $1S [X(e,hh)]_{n=1}$ exciton state is occupied at low excitation density, a fit with a simple Gaussian (dashed line), or Lorentzian according to Eq. (22) fails completely. In particular, the clearly visible high-energy Boltzmann tail is not accounted for. This pronounced

Boltzmann tail of the $[X(e,hh)]_{n=1}$ emission is observed in all our low-temperature experiments on single QW's. Obviously these observations cannot be explained by recombination of $\mathbf{K}=\mathbf{0}$ excitons, i.e., k is not conserved at low temperatures. The energy dispersion of the excitons has to be taken into account explicitly.

The translation invariance in the (x,y) plane is broken by the lateral potential fluctuations caused by the interface roughness, having amplitudes larger than the thermal energy kT_c of the excitons. As an example, for $\langle L_z \rangle = 5$ nm, the potential fluctuation due to a $\Delta L_z = 1$ monolayer of the mean well width in a GaAs/Al_{0.4}Ga_{0.6}As QW is $\Delta E \approx 7$ meV. The excitons thermalize and are laterally localized in the potential minima. Figure 4 visualizes this effect. The lateral localization of the "free" exciton within Δx gives rise to a **k** uncertainty $\Delta k \approx \hbar/\Delta x$. With increasing temperature the excitons delocalize and at RT ΔE is usually smaller than $kT_c = 26$ meV. **k** conservation is thus reestablished upon an increase in temperature as demonstrated by Fig. 3(a).

The transition from nonmomentum conserving recom-



FIG. 3. (a) Full line-shape analysis of room-temperature QW luminescence spectrum (dots). Solid line, including excitonic effects; dashed-dotted line, pure intersubband recombination. (b) Low-temperature QW luminescence spectrum (dots). Solid line, fit without k conservation. Dashed line, symmetrically (Gaussian) broadened K=0 exciton line. Hatched area, contribution due to $K \neq 0$ excitons.



FIG. 4. Schematic representation of lateral exciton energy distribution in the (x,y) plane: As long as the average thermal energy of the excitons is smaller than the amplitude of the energy fluctuations, i.e., $kT_c < \Delta E$, the excitons are localized in the potential minima.

bination of localized excitons to a momentum conserving one of delocalized excitons is a Mott transition.³⁷ The two types of excitons are separated by a boundary called the mobility edge. This edge, which is remarkably conclusive experimentally, has been observed by Hegarty *et al.*³⁸ in GaAs QW's using Rayleigh scattering and hole-burning experiments.

VII. CONCLUSION

Theoretical line shapes for interband and excitonic recombination in quantum wells are derived, including broadening due to final-state interaction and statistical broadening which might be caused by interface roughness and/or alloy fluctuations. Depending on growth conditions, which strongly influence the interface morphology, nearly Lorentzian or nearly Gaussian luminescence line shapes may be observed at low temperatures. Typical observations of both cases serve as examples. The influence of k conservation and of excitonic effects is discussed in detail. A comparison of experimental and theoretical line shapes of GaAs QW's at 300 K unambigously proves the predominant excitonic nature of the recombination involving only $\mathbf{K} = 0$ excitons, i.e., **k** is conserved. In contrast low-temperature spectra show clear evidence that k conservation is violated for small values of kT_c due to the thermalization and thus lateral localization of the excitons in potential fluctuations caused by mean well-width fluctuations. The transition from localized to delocalized exciton states presents a Mott transition.

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