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Trion Binding Energies and Wave Functions in Doped Quantum Wells

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The energy spectra of negative trions $(X^- = 2e + h)$ in one-sided doped GaAs quantum wells are calculated. The maps of the trion binding energy Δ as a function of well width w, electron concentration n, and the magnetic field B are obtained. The dependence of the trion ground state ("bright singlet" versus "dark triplet") on those parameters is established.

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1. Introduction

The photoluminescence (PL) spectra of two-dimensional electron gases (2DEGs) formed in doped quantum wells contain peaks corresponding to recombination of trions (charged excitons) X⁻ [1, 2]. The trion is a bound state of a pair of conduction electrons e and a valence (heavy) hole h. Whether trions can be considered as well-defined quasiparticles (with binding energy Δ and emission intensity τ^{-1} independent of the surrounding electrons), it depends on the 2DEG concentration n.

In the absence of a magnetic field, the PL spectrum as a function of n evolves from a trion peak to the "Fermi-edge singularity" [3]. The transition depends on the relation between the characteristic lengths or energies of the trion and of the 2DEG (Bohr radius $a_{\rm B}^*$ vs. $n^{-1/2}$, or Δ vs. Fermi energy).

In high magnetic fields B, the electrons fill only a fraction $\nu = 2\pi\lambda^2 n$ of the lowest Landau level (LL), and the trion radius scales with a magnetic length $\lambda = \sqrt{hc/eB}$. The "radius<distance" diluteness condition is equivalent to $\nu < 1$, suggesting [4] that the trions might remain bound even at n corresponding to

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 $\nu \sim \frac{1}{3}$, when electrons form an incompressible Laughlin liquid [5]. Indeed, a recent calculation [6] shows that emission from this state is due to the recombination of *fractionally* screened trions ("quasiexcitons").

The X⁻ spectra in empty wells [7, 8] are understood quite well. Several bound trion states (with a positive $\Delta = E_{\rm X} + E_{\rm e} - E_{\rm X^-}$) are distinguished by two-electron spin S and relative (with respect to the center of mass) angular momentum M. Only those trions with M = 0 are optically active (photon emission conserves M, and the left over electron has $M \equiv 0$). The most important states are [9–11]: "bright singlet" X⁻_{sb} with (S, M) = (0, 0), "dark triplet" X⁻_{td} (1, -1), "bright triplet" X⁻_{tb} (1, 0), and "dark singlet" X⁻_{sd} (0, -2). Depending on material, well width w, and magnetic field B, the ground state is either X⁻_{sb} or X⁻_{td}. The latter is favored by higher B, and in GaAs wells the singlet–triplet crossing occurs at B = 20 to 30 T.

The situation at larger concentrations is quite different. The understanding of emission from such states as Laughlin $\nu = \frac{1}{3}$ liquid is essential to establish PL as another (in addition to transport) probe of their microscopic properties [12, 13]. Therefore, most important is the *change* of the trion recombination compared to the empty well, possibly related to electron incompressibility. The trion immersed in a 2DEG is affected in two ways: (E1) The charge of confined electrons is compensated by a distant doping layer. The resulting electric field F penetrating the 2DEG forces the electrons and holes toward opposite walls of the well, weakening the e-h attraction compared to e-e repulsion within the trion, and thus affecting its binding. (E2) The trion is screened by the surrounding (mobile) electrons.

Only E2 is sensitive to the electron correlations. In Ref. [6] we show that the coupling of a trion to the Laughlin liquid depends on the particular trion wave function, leading (because of E1) to a qualitatively different behavior of PL at $\nu = \frac{1}{3}$ in different wells. Namely the emission energy is discontinuous only when the trion coupled to a 2DEG is the X_{td}^- (and not an X_{sb}^-).

The dependence of the trion ground state on w, n, and B is addressed in this note. We report realistic, exact-diagonalization calculations of the X⁻ binding energy in GaAs/AlGaAs wells doped on one side, taking into account E1. The results prove that the effect of F on X⁻ recombination (E1) is significant and must be accounted for when interpreting the PL spectra in terms of trion-2DEG coupling (E2). They should also help to design structures suitable for the PL studies of incompressible electron liquids.

2. Model

In numerical calculations we use spherical geometry [14]. The monopoly strength defined in the units of flux quantum as $2Q(hc/e) = 4\pi R^2 B$, the total magnetic flux through a sphere of radius R (equivalently, $Q\lambda^2 = R^2$). The LLs have the form of degenerate angular momentum shells with $l \ge Q$.

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The e and h densities $\varrho(z)$ are calculated self-consistently [15] as a function of w and n. Two sample results are shown in Fig. 1, showing splitting of e and h layers in the wider well. These densities are used in the calculation of e–e and e–h Coulomb matrix elements. The Δ s are obtained from diagonalization of 2e + h and e + h Hamiltonians for several values of $2Q \leq 30$. Five LLs for both e and h are included, and the hole cyclotron energies are from Ref. [16]. In Fig. 2 we plot Δ as a function of squared surface curvature $(\lambda/R)^2 = Q^{-1}$, for X_{sb}^- and X_{td}^- in a w = 20 nm well with $n = 2 \times 10^{11}$ cm⁻² and B = 25 T. Regular dependence allows accurate (quadratic) extrapolation of the binding energies to the $\lambda/R = 0$ limit.



Fig. 1. Band energy and carrier density profiles along normal (z) direction for w = 10 nm (a) and 20 nm (b) GaAs wells, doped on one side to $n = 2 \times 10^{11}$ cm⁻².

The values of Δ plotted in this and the following plots do not include the electron Zeeman energy $E_{\rm Z}^{\rm e}$, which must be subtracted from Δ to give the binding energy of singlet states. In PL spectrum, the sum $E_{\rm Z}^{\rm e} + E_{\rm Z}^{\rm h}$ splits the peaks for ω_+ and ω_- polarizations, but the splitting between the corresponding peaks for different trions is (for constant $E_{\rm Z}$ s) unaffected.

3. Results and discussion

The extrapolated binding energies of all four trions are compared in the next four plots. Motivated by a recent experiment of Byszewski et al. [13], for a reference system we choose parameters of Fig. 2, for which the Laughlin $\nu = \frac{1}{3}$ state occurs at a high, but experimentally accessible *B*.

In Fig. 3, w and n are constant and B varies from 10 to 50 T. Neglecting Zeeman energy, the X_{sb}^- crosses X_{td}^- at $B \approx 10$ T and unbinds at $B \approx 30$ T in this well. Assuming $E_Z^e \sim 0.2$ meV [11], the only bound trion at $B \ge 20$ T is X_{td}^- with $\Delta \approx 0.8$ meV. It is the ground state in the whole $\nu < 1$ regime.

In Fig. 4, w and B are constant, while n changes from 0 to 3×10^{11} cm⁻². Clearly, the X_{sb}⁻ looses binding energy more rapidly than X_{td}⁻ as a function of n. This is responsible for the shift of the singlet-triplet crossing to lower B in doped wells compared to the earlier estimates [11]. Remarkably, the (triplet) trion has $\Delta > 0.5$ meV ~ 5 K even at a very large n.

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Fig. 2. Trion binding energies Δ as a function of squared surface curvature $(\lambda/R)^2$. Fig. 3. Trion binding energies Δ as a function of magnetic field B.



Fig. 4. Trion binding energies Δ as a function of concentration n. Fig. 5. Trion binding energies Δ as a function of well width w.

In Fig. 5, n and B are constant, and w varies from 10 to 30 nm. The X_{sb}^- is the ground state in narrow wells, crossing the X_{td}^- at $w \approx 15$ nm (neglecting E_Z). Knowing that emission from a trion coupled to a 2DEG shows discontinuity at $\nu = \frac{1}{3}$ only when this trion is an X_{td}^- [6], we find that wells with w = 15 to 25 nm are most suitable for PL studies of Laughlin incompressibility. The 20 nm well used in Ref. [13] seems ideal by having X_{td}^- s with a large $\Delta \sim 0.8$ meV and no other bound trions.

Figure 6 is an example of a map of $\Delta(n, B)$ for a constant w. The energy contours are only shown for X_{sb}^- and X_{td}^- , and the grey and white areas indicate two different ground states. The dependence of the singlet-triplet transition on B and n is evident, and the crossing of the ground state boundary with the $\nu = \frac{1}{3}$ line is found at $n \approx 1.2 \times 10^{11}$ cm⁻² (neglecting E_Z).

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Fig. 6. Trion binding energies Δ as a function of concentration n and magnetic field B. Energy contours of X_{sb}^- and X_{td}^- are shown with dashed and solid lines.

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