Single nitrogen dyad magnetoluminescence in GaAs

S. Marcet,[1] C. Ouellet-Plamondon,[1] J. F. Klem,[2] and S. Francoeur[1,*]
[1]*Département de Génie Physique, Ecole Polytechnique de Montréal, Montréal, Québec, Canada H3C 3A7*
[2]*Sandia National Laboratories, Albuquerque, New Mexico 87185, USA*
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We report on the excitonic luminescence from two nearby nitrogen atoms (a dyad) in GaAs with and without an external magnetic field. The data are analyzed using a Hamiltonian taking into account the effects of the exchange interaction, the crystal field, and the Zeeman interaction and allowing the evaluation of the relative oscillator strength of the optical transitions and their polarization. Without the external magnetic field, we determine the exchange and crystal-field parameters characterizing the four excitonic states observed from dyads oriented along [110] or $[1\bar{1}0]$ and find that it is necessary to reduce the symmetry of all the terms involved in the Hamiltonian to the symmetry of the dyads (C_{2v}). As expected from two smaller atoms, the parameters indicate a dyad under tensile strain. Although the degeneracy of all excitonic states is already lifted, the magnetic field allows a closer examination of the nature of these states. The small diamagnetic shift of 1.99 ± 0.06 μeV T^{-2} is consistent with a strong localization of the electron to the nitrogen dyad and the g factor of the electron is an intermediate value between that of a free electron in GaAs and a perfectly localized electron.

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I. INTRODUCTION

Recently, probing single isoelectronic impurity centers in semiconductors has been achieved.[1] This has revealed critical information on their electronic properties, their symmetry, and their distinctive signature that would have been otherwise masked by ensemble averaging. First observed a few decades ago,[2] the characteristics of these centers, formed from a few impurities, are in many aspects an interesting alternative to conventional semiconductor quantum dots. For example, the inhomogeneous broadening of the energy of isoelectronic impurity centers as a function of the atomic separation or the number of atoms involved is relatively large (>10 meV) making it easy to discriminate between various configurations and match the emission energy with the modes of a resonator.[3] The generation of triggered single photons from single impurity centers has interesting applications in the field of quantum information.[4–6] Furthermore, in contrast to self-assembled quantum dots composed of a large number of atoms, so far the most studied candidate for quantum light sources, the symmetry of isoelectronic centers is very well defined and directly suitable for the generation of entangled photons via a biexcitonic cascade.[7]

In this work, we analyze the fine structure splitting of the emission lines related to single nitrogen dyads in GaAs to better understand their electronic structure determined by the interplay of the exchange interaction, the crystal field associated with the symmetry of the defect, and the effects of an external magnetic field. All experimental results are modeled using a perturbation Hamiltonian allowing the calculation of the energy and the relative oscillator strength of the excitonic transitions. Preliminary results under magnetic field have been published but no detailed analysis has been developed yet.[8]

A nitrogen atom on an anionic site of GaAs is an isovalent impurity. In contrast to most isovalent impurities, its strong electronegativity and the important lattice distortion it generates create a short-range confinement potential that can trap an electron. This electron attracts, via Coulombic interaction, a weakly bound hole, thereby forming excitonic bound states in the forbidden gap of GaAs.[9–11] At dilute nitrogen doping, two photoluminescent centers referred to as X_1 and X_2 and originating from two distinct dyad configurations can be observed.[1] Their exact configuration has not yet been established but they correspond to pair arrangements of C_{2v} symmetry where the two nitrogen atoms are most likely first or second anionic neighbors along the [110] direction. States associated with other dyad configurations are located above the GaAs conduction band minimum and are observable only through the application of hydrostatic pressure.[12] In this work, we focus on the high energy center labeled X_1.

In Sec. II, we briefly describe the sample used and the experimental procedure. Section III explains the perturbation Hamiltonian for the bound excitons and the formalism used to model our data. Sections IV and V show the experimental data at zero field and under a magnetic field in Faraday configuration, respectively, and the results of the simulation.

II. SAMPLE AND EXPERIMENTAL SETUP

The sample used, grown by molecular beam epitaxy, consists of a 25 nm layer of N-doped GaAs, clad by a protective 5 nm GaAs layer on both sides and placed between two barriers of $Al_{0.25}Ga_{0.75}As$. The nitrogen concentration of 3×10^5 μm^{-2} corresponds to a dyad area density of 0.6 μm^{-2}.[1]

Samples were cooled to 4.5 K in a liquid helium cryostat and the photoluminescence (PL) measurements were made using a custom-made confocal microscope. The sample positioners and microscope objective are inside the cryostat and the remaining optics are located outside at its top.[13] The temperature and mechanical stability of this confocal microscope allow studying the same emitter for more than 10 h without any noticeable drift of the sample.

A cw-laser beam at 782 nm is brought to the microscope by a 5 μm-core polarization maintaining optical fiber, partially reflected to the cryostat using an asymmetrical beam splitter ($R=8\%$, $T=92\%$), and focused on the surface of the sample with an aspherical lens ($f=3.1$ mm). The full width at half maximum of the excitation spot at the surface of the sample is 0.78 μm. The PL emitted from the sample is collected using the same aspherical lens, transmitted by the beam splitter, and coupled to a 5 μm-core polarization maintaining optical fiber. The core of the fiber acts as a confocal aperture and provides a spatial resolution of 0.82 μm. Considering the surface density of nitrogen dyads, this resolution is sufficient to easily study the PL from a single emitter. The emission spectra are measured using a spectrometer and a charge coupled device camera providing a spectral resolution of 60 μeV. The polarization of the luminescence is analyzed using a motorized $\lambda/2$ wave plate and a polarizer placed just before the collection fiber. The cryostat tail is inserted in the bore of a superconducting coil magnet providing a magnetic field up to 7 T in a Faraday configuration.

III. HAMILTONIAN

The Hamiltonian describing an exciton bound to a nitrogen dyad under an external magnetic field can be written as[10]

$$H = H_{\mathrm{EX}} + H_{\mathrm{CF}} + H_Z. \tag{1}$$

In the following analysis, we consider the spin-orbit interaction strong enough to neglect the split-off excitons located at higher energies ($\sim$341 meV). However, in contrast to most quantum dot systems, light and heavy holes must be considered simultaneously.

The first term, H_{EX}, describes the exchange interaction between an electron and a hole, which we assume to be isotropic by neglecting higher order terms other than

$$H_{\mathrm{EX}} = -a\mathbf{J}\cdot\mathbf{S}, \tag{2}$$

where $\mathbf{J}$ and $\mathbf{S}$ represent the total angular momentum of the hole and the spin of the electron, respectively. The parameter a is to be determined experimentally, but it should be positive to position the quintuplet at lower energy. The crystal field does not influence electron states and its effects on the hole states can be written as[10]

$$H_{\mathrm{CF}} = -D\left[J_z^2 - \frac{1}{3}J(J+1)\right] - E(J_x^2 - J_y^2), \tag{3}$$

where the z axis is taken along the nitrogen atoms forming the dyad [110], and x and y are taken along $[\bar{1}10]$ and [001], respectively, and $J(J+1)$ is the eigenvalue of the J^2 operator for a hole with $J=3/2$. The parameter D describes the perturbation along the dyad axis and should be positive for a dyad in tension and negative in compression.[14] Due to the relatively short Ga-N bond length, the nitrogen dyad in GaAs is in tension and therefore we expect D to be positive. The parameter E, which describes the perturbation tangential to the dyad axis, will be determined experimentally. The value of the parameter D is expected to be larger than E because the axial part of the crystal field should dominate over the influence of the surrounding atoms.[10]

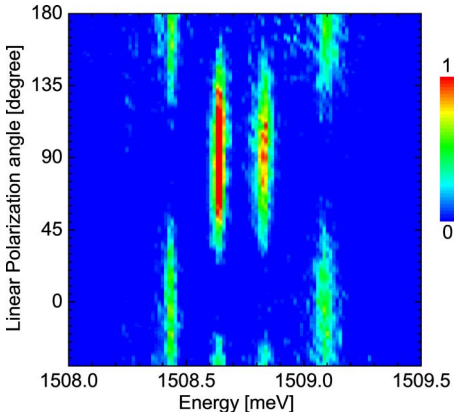

FIG. 1. (Color online) PL from a single nitrogen dyad as a function of emission energy and linear polarization angle. Two optical transitions are linearly polarized along z (0°) and the remaining two are polarized perpendicularly along x (90°). Only four transitions are observed confirming that the dyad is located in the plane of the sample (x-z plane).

The last term of Eq. (1) describes the Zeeman interaction of the bound exciton with the external magnetic field B. It consists of the usual linear Zeeman term along with a quadratic term accounting for the diamagnetic shift,

$$H_Z = \mu_{\mathrm{B}}\left[g_e\mathbf{B}\cdot\mathbf{S} + K\mathbf{B}\cdot\mathbf{J} + L\sum_{i=x,y,z} J_i^3 B_i\right] + CB^2, \tag{4}$$

where μ_{B} is the Bohr magneton, g_e is the g factor of the bound electron, K and L are the isotropic and anisotropic interactions for the hole, and C is the diamagnetic shift constant of the exciton.

The total Hamiltonian, H, representing the interactions of the eight excitonic states with themselves or with an external perturbation, takes the form of an 8×8 matrix constructed from the Kronecker product of angular momentum matrices for $J=3/2$ and $S=1/2$. The eigenvalues of this Hamiltonian represent the energy of the eight exciton eigenstates. It is possible to know which of those states are optically allowed by computing their relative oscillator strengths using the standard equation for transition probabilities, $|\langle\phi_i|\vec{Q}|\phi_g\rangle|^2$, where $\vec{Q}$ is the electric dipole operator, ϕ_i is the initial state, and ϕ_g is the vacuum state.[10] This vectorial definition allows calculating the relative transition probabilities for different polarization orientations with respect to the dyad. Although these Hamiltonians have been successfully used to model the excitonic states of nitrogen dyads in GaP,[11] they can be significantly improved, as will be discussed later, by fully accounting for the C_{2v} symmetry.

IV. ZERO-FIELD MEASUREMENTS

The PL spectrum of a nitrogen dyad as a function of the emission linear polarization is shown in Fig. 1. From this intensity map, we identify two pairs of emission peaks orthogonally polarized with respect to each other. For this dyad of C_{2v} symmetry,[1] two of the eight possible optical transitions are forbidden and the number of transitions observed

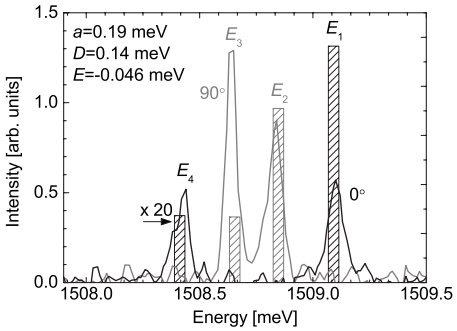

FIG. 2. PL spectra from a single nitrogen dyad for polarization angles of 0° and 90°. The dashed rectangles show the result of a calculation using Eqs. (2) and (3), with the height indicating the calculated relative oscillator strength. For the peak labeled E_4, the relative oscillator strength is multiplied by 20 to make it visible in the figure. The inset shows the values of the parameters used for the calculation.

can either be four or six depending on the orientation of the dyad with respect to the wave vector of the detected photons. The results presented here correspond to a dyad located in the plane of the sample (x-z plane), and, in this particular configuration, only four of the remaining six transitions can be observed. The transitions are linearly polarized along (z) or perpendicular (x) to the dyad.

Figure 2 shows two PL spectra corresponding to polarization angles of 0° and 90°. Also shown is the energy and the relative oscillator strength of the optical transitions calculated from a Hamiltonian combining Eqs. (2) and (3). The optical transitions E_1 and E_4 (E_2 and E_3) are polarized along (perpendicular to) the N dyad in the (001) plane. As can be observed, the parameters listed in the inset of Fig. 2 accurately reproduce the energy positions of the four emission lines. These particular values were obtained by minimizing the energy separation between the calculated and measured peaks, $\Delta E=\sqrt{\Delta E_1^2+\Delta E_2^2+\Delta E_3^2+\Delta E_4^2}$. The minimum value for ΔE as a function of the parameter a is shown in Fig. 3 with the corresponding value for D and $-E$ for each point. We

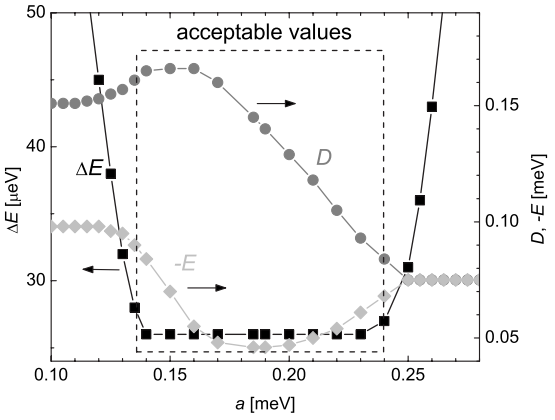

FIG. 3. Evolution of the error ΔE as a function of the parameter a (in black). Also shown are the corresponding values for D and $-E$ that minimized ΔE (in gray and light gray). The dashed rectangle represents a region for which the error is minimum and equal to 26 μeV.

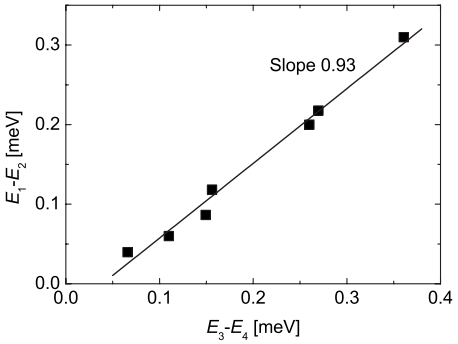

FIG. 4. Ratio of the energy differences of the first two peaks (E_1-E_2) with the other two (E_3-E_4) for various nitrogen dyads. Although the energies vary for different dyads, this ratio is constant for each of them. The line shows the linear regression with a slope of 0.93.

determine a region of acceptable values for the fitting parameters when ΔE is minimum (26 μeV), which for a occurs between 0.14 and 0.24 meV. The center of this region was chosen as the value for a with its corresponding value for D and E. Also, we use this region to determine an area of validity for D (between 0.084 and 0.166 meV) and E (between −0.046 and −0.09 meV). As expected, the signs of those parameters are consistent with the considerations discussed in Sec. III. We find a value $a=190\pm50$ μeV for the e-h exchange interaction, which is smaller than the value reported in GaP ($a\approx0.5$ meV).[9,10] This smaller value can be explained by a larger exciton radius in GaAs leading to a smaller wave function overlap and a weaker e-h exchange interaction.[15]

It is not possible to directly compare the values obtained from the relative oscillator strength calculation with the measured PL intensity due to the thermalization of carriers, but they are a reliable indicator of the allowed transitions and the polarization of the emission lines with respect to the orientation of the dyad. As expected, four of the eight lines are obtained in this particular configuration. Finally, the fact that there is more oscillator strength for the states at a higher energy probably indicates a significant population transfer to a lower energy state.

Strong similarities between all nitrogen dyads located in the x-z plane were observed. For example, the polarization of the two center peaks (labeled E_2 and E_3 in Fig. 2) is always orthogonal to the polarization of the two others (labeled E_1 and E_4). Although this polarization rule is always observed, the energy differences between each level somewhat vary for each dyad indicating the influence of the local environment on the excitonic states. However, the ratio of the energy differences of E_1-E_2 with E_3-E_4 is remarkably constant for all measured dyads as shown in Fig. 4. This ratio of 0.93 is slightly lower than the value of one predicted with the model presented in Sec. III. These observations imply that (1) this ratio is an intrinsic property of this dyad family and that it is independent of the local environment and (2) the current model fails to reproduce a characteristic observed on all dyads.

We refine our model by fully accounting for the C_{2v} symmetry in the H_{EX} and H_{CF} Hamiltonians. Reducing the sym-

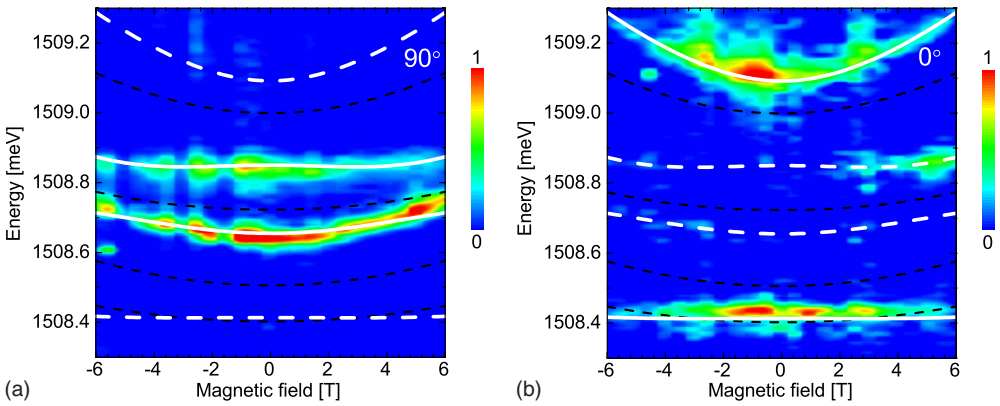

FIG. 5. (Color online) PL intensity (color scale) as a function of magnetic field and emission energy for linear polarizations along and perpendicular to the dyad (0° and 90°, respectively). Solid (dashed) white lines show the calculated positions of the allowed optical transitions in the observed (perpendicular) polarization. Black dashed lines show the forbidden optical transitions.

metry of H_{EX} from that of the host crystal T_d to that of the nitrogen dyad C_{2v}, the exchange Hamiltonian becomes

$$H_{\mathrm{EX}} = -\sum_{i=x,y,z} a_i J_i S_i,$$

and, as expected from an orthorhombic system, requires three independent parameters. The crystal-field Hamiltonian of Eq. (3) proposed in Ref. 11 is based on the assumption that the three required crystal-field parameters F_x, F_y, and F_z are not mutually independent.[16] It was assumed that $\Sigma_{i=x,y,z} F_i = 0$ leading to the following relations: $F_x = \frac{D}{3} - E$, $F_y = \frac{D}{3} + E$, and $F_z = \frac{-2D}{3}$. Without this simplifying assumption, the C_{2v} crystal-field Hamiltonian becomes

$$H_{\mathrm{CF}} = \sum_{i=x,y,z} F_i J_i^2.$$

Using these two Hamiltonians, the calculated ratio $(E_2 - E_1)/(E_4 - E_3)$ better fits the experimental data of Fig. 4 and the error ΔE is reduced from 26 to 0.66 μeV showing an important improvement of the model by using the following parameters:

$$a_x = 217\ \mu\mathrm{eV}, \quad a_y = 161\ \mu\mathrm{eV}, \quad a_z = 166\ \mu\mathrm{eV},$$

$$F_x = 96\ \mu\mathrm{eV}, \quad F_y = 2.8\ \mu\mathrm{eV}, \quad F_z = -96\ \mu\mathrm{eV}.$$

It is interesting to note that a_x is significantly larger than the two other parameters. Since the exchange interaction is proportional to the overlap between the electron and hole wave functions, these parameters could allow the determination of the absolute orientation of the dyad and the precise identification of excitonic states. A detailed study is underway. Finally, in the context of the results presented in this section, it appears necessary to fully account for the C_{2v} symmetry in both the exchange interaction and the crystal field to get a satisfactory agreement with the experimental data and to get a representative picture of the physics involved.

V. ZEEMAN EFFECT

In this section, we analyze the evolution of the excitonic state energies as a function of an external magnetic field applied in Faraday configuration perpendicular to the surface of the sample and to the N dyad axis orientation. Figure 5 shows the PL intensity polarized along and perpendicular to the dyad as a function of the emission energy and the external magnetic field. Since all degeneracies were already lifted by the *e-h* exchange interaction and the crystal field, no additional splitting is expected under a magnetic field in C_{2v} symmetry. However, as can be seen from Fig. 5, the field induces an energy shift of all four transitions and a slight depolarization of E_2. The decrease in the emission intensity is not explained at this point.

We begin by analyzing the diamagnetic shift common to all four transitions. This shift is obtained by calculating $\frac{1}{4}\Sigma_{i=1}^{4} E_i(B) - E_i$ and is plotted in Fig. 6. As expected, the shift is clearly quadratic with the magnetic field and a diamagnetic coefficient of 1.99 ± 0.06 μeV T^{-2} is obtained. This small value is typical of a strong localization of the carriers forming the exciton.

The measured diamagnetic shift coefficient can be used to estimate the localization of the electron of the nitrogen dyad.

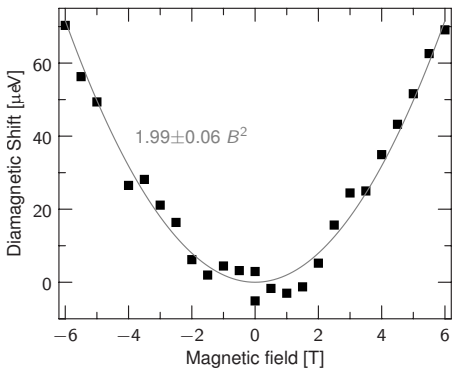

FIG. 6. Diamagnetic shift calculated from the averaged energy difference of the four observed transitions with respect to the zero-field position. The gray line represents a quadratic fit with a coefficient of 1.99 μeV T^{-2}.

The diamagnetic shift of two confined particles without Coulomb interaction can be written as[17]

$$C = \frac{e^2}{8}\left(\frac{\langle r_e^2\rangle}{m_e} + \frac{\langle r_h^2\rangle}{m_h}\right) = C_e + C_h, \tag{5}$$

where m_h and m_e are the usual carrier effective masses and $\langle r_h^2\rangle^{1/2}$ and $\langle r_e^2\rangle^{1/2}$ are the average radii of the localization region of the hole and electron. Although this expression was derived for strongly confined carriers, we assume that the hole wave function radius is that of a hole bound to an acceptor via Coulombic interaction. For a hole of average effective mass $m_h=0.2m_0$, its radius is 3.4 nm. Then, according to the previous equation, the hole diamagnetic shift should be $C_h=1.27$ μeV T^{-2} leaving a shift of $C_e=0.72$ associated with the electron. From this value, we estimate the electron's radius at 16.2 Å using $m_e=0.08m_0$. Although an approximate value, this estimate reveals the significant localization of the electron wave function in agreement with the Hopfield-Thomas-Lynch (HTL) model.[18] Furthermore, a full width at half maximum of about 6 Å has been calculated for an electron bound to an isolated nitrogen atom.[19] Taking into account that we have a center composed of two atoms and that the hole bound to the electron increases the kinetic energy of the electron, this agrees well with the value observed.

To model the effects which are linear with the magnetic field, a fit of the energy of all four emission lines is performed as a function of the three parameters g_e, K, and L. In the HTL model for a relatively delocalized effective-mass-like bound hole state, the parameter K should be close to the value of a hole in GaAs, $K=-0.5\pm0.1$.[20,21] All exchange and crystal-field parameters presented in the previous section are kept constant. Again, the error ΔE is calculated and summed over each transition and each magnetic field value:

$$\Delta E = \sqrt{\sum_{i=1}^{4}\sum_{B=-6}^{6}[E_i^{\mathrm{meas}}(B) - E_i^{\mathrm{cal}}(B)^{\mathrm{cal}}]^2}. \tag{6}$$

The minimum value, $\Delta E=108$ μeV, is obtained with $g_e=0.82$, $K=-0.42$, and $L=0.1$. The calculated energy of the eight excitonic transitions as a function of the magnetic field is shown in Fig. 5, where the bright and dark lines represent the allowed and forbidden transitions, respectively. As can be seen, the model adequately reproduces the energy and polarization of the observed transitions. Although this represents the best set of parameters, we find that it is possible to obtain a relatively good fit for a range of values. For example, using ΔE within 10% of the minimum ($\Delta E \leq 119$ μeV) as the criterion for a satisfactory fit, we would get the following ranges of acceptable values:

$$g_e \in [0,\ 0.94],$$

$$K \in [-0.4,\ -0.6]$$

(Refs. 20 and 21), and

$$L \in [-0.02,\ 0.18].$$

This validates the assumption on parameter K and, as expected for a relatively delocalized hole state, the anisotropy parameter L is smaller than K. The g factor for the electron, g_e, is found to be between 0 and 0.94. This is smaller than the value 1.85 found in GaP.[22] The range of possible values for an electron in GaAs would be between 2 for a perfectly localized electron and −0.44 for a free electron.[23] Although it is difficult to quantitatively correlate g_e with the localization of the electron, this might indicate that the electron bound to a nitrogen dyad is less strongly localized in GaAs than in GaP, which was confirmed by the diamagnetic shift analyzed above.

VI. CONCLUSION

In this work, we have presented a study of the magneto-photoluminescence of the excitonic states bound to a single nitrogen dyad in GaAs. Zero-field spectra were analyzed by calculating the energy and relative oscillator strength of the excitonic levels from an exchange interaction and crystal-field Hamiltonians. A simple model replicates the energy and polarization of the optical transitions,[10] but a detailed analysis of several nitrogen dyad shows the necessity of refining the model by fully accounting for the C_{2v} symmetry. Zeeman effect in Faraday configuration is analyzed by including in the Hamiltonian a linear Zeeman term and a quadratic dependence accounting for the diamagnetic shift. The fitting parameters and the diamagnetic shift are consistent with the HTL bound exciton model with a relatively delocalized effective-mass-like bound hole state and a significantly more localized electron state. This study shows a larger exciton radius and a less localized electron state in GaAs than in GaP.

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*sebastien.francoeur@polymtl.ca

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