

Magnetoexcitons in anisotropic semiconductors

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Using a numerical technique, we have calculated the exciton ground state in a uniaxially anisotropic semiconductor with and without the presence of a magnetic field. Numerical results are given for the exciton energy level as a function of magnetic field for a wide range of anisotropy parameters $0.001 \leq \alpha\beta \leq 1000$ and effective field $0 \leq \gamma \leq 10$. We have demonstrated that by fitting the experimental data of the field dependence, in a proper field range, with the field aligned in the direction of the uniaxis, the exciton in plane reduced mass μ_{\perp} and the parameter $\alpha\beta$ can be obtained simultaneously. As an example, magnetoluminescence of ordered GaInP₂ measured in the field range $B \leq 14$ T is analyzed by applying this method. Analytical formulas have been found for calculating exciton binding energy and the related variational parameters for a well-known method with trial function $f(x, y, z) = (\pi a^2 b)^{-1} \exp[-\sqrt{(x^2 + y^2)/a^2 + z^2/b^2}]$. Various approximate approaches for calculating the exciton binding energy and the magnetoexciton states are discussed and compared. © 1998 American Institute of Physics. [S0021-8979(98)02301-9]

I. INTRODUCTION

Excitonic states in an anisotropic semiconductor and their behavior in a magnetic field have been investigated extensively in the past forty years. In a semiconductor with cubic symmetry, the anisotropy for a direct exciton occurs mainly from the anisotropy of the effective mass tensor of the valence band. Exciton states in cubic semiconductors with and without a magnetic field have been studied by, for examples, Dresselhaus,¹ Altarelli and Lipari,² Swierkowski,³ Cho *et al.*,⁴ and Lipari and Altarelli.⁵ Degeneracy combined with the anisotropy causes a strong mixing of states and results in a complicated magnetic field dependence of the excitonic states.²⁻⁵ On the other hand, excitonic states in semiconductors with uniaxial symmetry are relatively easy to deal with. When a large valence band splitting exists in a semiconductor, for instance, in crystals like CdS⁶ and CdSe⁷ with Wurtzite symmetry, in semiconductor quantum wells and superlattices⁸ or in cubic semiconductors subjected to a high uniaxial stress along the [001] or [111] direction, an ellipsoid energy dispersion is a good approximation for the electronic states near $\mathbf{k}=0$. Thus, excitonic states are the solutions of a single effective mass equation with anisotropic masses and maybe anisotropic dielectric constants as well. We refer to this type of anisotropic exciton as a simple anisotropic exciton, compared to the more complicated situations in cubic semiconductors.

For a simple anisotropic exciton or a similar problem for shallow impurities, there have been various perturbative methods proposed for calculating its eigenstates. For instances, trial-wave function or basis-expansion methods were used by Kittel and Mitchell,⁹ Kohn and Luttinger,¹⁰ Faulkner,¹¹ and Baldereschi and Diaz,¹² and a method of solving a set of coupled radial equations was used by Broeckx *et al.*¹³

For the simple anisotropic exciton in a magnetic field aligned along the symmetric axis, the effects of the anisotropy and field are in fact similar in terms of symmetry. Perturbative methods have been used to obtain the exciton states in a weak field for materials with rather weak anisotropy, like CdS by Hopfield and Thomas⁶ and CdSe by Wheeler and Dimmock.⁷ Variational methods have also been used for solving the problem, for instance, a one-parameter trial Hamiltonian method by Dai *et al.*¹⁴ which is only good for a weak field and weak anisotropy, and a basis-expansion method by Twardowski and Jinter¹⁵ which is more accurate for a strong field and excited states than for a weak field and ground state. Very recently, Lee and Lee¹⁶ proposed a method to treat the anisotropic magnetoexciton as an isotropic one with an effective interaction constant, when the anisotropy is not too strong.

The motivation of this work is to interpret the magnetoluminescence data of ordered III-V alloys, GaInP₂ in particular,¹⁷ in an intermediate field range in which the perturbative approach is not valid any more. The ordering changes the crystal structure from zinc-blende to CuPt, and causes an effective mass anisotropy in the conduction band and a splitting of the degenerate valence band. As a good approximation, both the conduction band and the topmost valence band have ellipsoid energy dispersions.¹⁸ Also, it is of a general interest to understand the magnetoexciton with an arbitrary anisotropy and magnetic field, but without the complicated valence band structure of cubic semiconductors.

For an isotropic exciton, its magnetic field dependence has been very well studied, in the pioneering work of Yafet *et al.*¹⁹ using a trial function with a form $\exp[-az^2 - b(x^2 + y^2)]$ and in work by others using improved or more sophisticated trial functions, for instance, Larsen,²⁰ Pokatilov and Rusanov,²¹ and Gerlach *et al.*,²² and using other techniques: perturbation methods by Ruder *et al.*,²³ Pavlov-Verevkin and Zhilinskii,²⁴ and Cohen and Herman,²⁵ solving multiple radial equations by Cabib *et al.*,²⁶ and basis-expansion meth-

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ods by Aldrich and Greene²⁷ and Makado and McGill.²⁸ For the isotropic magnetoexciton, the numerical results for experimentally accessible fields are usually tabulated,^{19–28} which makes it possible to use them for analyzing the experimental results. However, for the anisotropic magnetoexciton, such kinds of tables are not available, to the best of our knowledge. On the other hand, in the early works,^{6,7} as well as in our recent work,¹⁷ in order to obtain the exciton reduced masses in the directions parallel and perpendicular to the uniaxial, measurements including the excited states and/or with two field orientations were required. Strictly speaking, it is not possible to obtain the two reduced masses by analyzing the two-field data because the field dependence of the exciton state is not just simply a function of the two reduced masses, but rather of the individual electron and hole effective masses. Only in the low-field limit, can the diamagnetic shifts be described by the relatively simple functions which contain only the two reduced masses.^{6,7,17} Very often, such a low-field limit gives a very small field range in which diamagnetic shift is at first rather small and second could be affected by the exciton localization caused by certain fluctuations. Also, it is not trivial to decide in what field range the formalism for the diamagnetic shift is a good approximation.

In this work, we choose to extend the numerical method of Ref. 26 for the isotropic exciton to the anisotropic exciton. We are able to achieve an accuracy of four or five digits below the decimal point in calculating the exciton binding energy or its magnetic shift in the anisotropy range $0.001 \leq \alpha\beta \leq 1000$ and in the field range $0 \leq \gamma \leq 10$ ($\alpha\beta$ and γ are defined below), at least for the exciton ground state. We will demonstrate how to obtain the exciton reduced mass and the anisotropy parameter $\alpha\beta$ simultaneously by fitting the magnetoluminescence data to the theoretical results. A few fairly simple analytical formulas are found for the long existing approximate approaches for the exciton binding energy. Also, the applicability and the accuracy of various approximations are discussed.

II. FORMALISM AND RESULTS

A. Magnetic field $\mathbf{B}=\mathbf{0}$

The electron-hole relative motion of an excitonic state can be described by the following equation in a “simple-anisotropic-exciton” model:^{1,6,29}

$$\left(-\frac{\hbar^2}{2\mu_{\perp}} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{\hbar^2}{2\mu_{\parallel}} \frac{\partial^2}{\partial z^2} - \frac{e^2}{\sqrt{\epsilon_{\perp} \epsilon_{\parallel} (x^2 + y^2) + \epsilon_{\perp}^2 z^2}} \right) \psi = E\psi, \quad (1)$$

where $\mu_{\perp}(\epsilon_{\perp})$ and $\mu_{\parallel}(\epsilon_{\parallel})$ are exciton reduced masses (dielectric constants) in the directions perpendicular and parallel to the symmetry axis, respectively. In Eq. (1), the zero of the energy has been chosen as the band gap.

If we define a mean dielectric constant $\epsilon_0 = \sqrt{(\epsilon_{\perp} \epsilon_{\parallel})}$, a mass anisotropy $\alpha = \mu_{\perp} / \mu_{\parallel}$, a dielectric anisotropy $\beta = \epsilon_{\perp} / \epsilon_{\parallel}$, and a transformation $z' = z\sqrt{\alpha}$, use the effective

Rydberg $R_{\perp} = \mu_{\perp} e^4 / (2\hbar^2 \epsilon_0^2)$ and the effective Bohr radius $a_{\perp} = \hbar^2 \epsilon_0 / (\mu_{\perp} e^2)$ as units for energy and length, respectively, Eq. (1) becomes

$$\left(-\frac{\partial^2}{\partial x'^2} - \frac{\partial^2}{\partial y'^2} - \frac{\partial^2}{\partial z'^2} - \frac{2}{\sqrt{x'^2 + y'^2 + \alpha\beta z'^2}} \right) \psi = E\psi. \quad (2)$$

Transforming Eq. (2) to spherical coordinates (r, θ, φ) , we have⁷

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{L^2}{r^2} - \frac{2}{r\sqrt{1 - (1 - \alpha\beta)\cos^2 \theta}} \right) \psi = E\psi, \quad (3)$$

where L is the angular momentum operator.

The Hamiltonian in Eq. (2) has an axial symmetry about z as well as an inversion symmetry, therefore both the z component of angular momentum m and parity are good quantum numbers. We are only interested in the eigenstates with $m=0$ and even parity, because only these states have nonzero matrix elements for band-edge optical transitions. As in Ref. 26, we can express $\psi(r)$ as a combination of spherical harmonics $Y_{\ell m}$ with even ℓ and $m=0$;

$$\psi(r, \theta) = \sum_{\text{even } \ell} F_{\ell}(r) Y_{\ell 0}(\theta, \varphi). \quad (4)$$

Substituting Eq. (4) into Eq. (3), we obtain a set of coupled differential equations for the radial functions $F_{\ell}(r)$:

$$\sum_{\text{even } \ell'} H_{\ell \ell'} F_{\ell'}(r) = E F_{\ell}(r), \quad (5)$$

where

$$H_{\ell \ell'} = \left(-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{l(l+1)}{r^2} \right) \delta_{\ell \ell'} - \frac{2}{r} u_{\ell \ell'}, \quad (6)$$

and

$$u_{\ell \ell'} = \langle Y_{\ell' 0} | \frac{1}{\sqrt{1 - (1 - \alpha\beta)\cos^2 \theta}} | Y_{\ell 0} \rangle.$$

To solve Eq. (5) numerically, we follow Ref. 26 by introducing a transformation

$$r = \frac{k\xi}{(1-\xi)},$$

with $0 < \xi < 1$. The scale factor k can be adjusted to give a good representation of the range where the wave function is important (typically k is chosen between 0.4 to 2).

Defining

$$f_{\ell}(\xi) = \xi F_{\ell}(r),$$

Eq. (5) becomes

$$\sum_{\text{even } \ell'} \left[\left(-\frac{(1-\xi)^4}{k^2} \frac{d^2}{d\xi^2} + \frac{(1-\xi)^2 \ell(\ell+1)}{k^2 \xi^2} \right) \delta_{\ell \ell'} - \frac{2(1-\xi)}{k\xi} u_{\ell \ell'} \right] f_{\ell'} = E f_{\ell}, \quad (7)$$

which is a set of differential equations for $f_{\ell}(\xi)$'s. We, then, solve these equations by using a finite difference method,

TABLE I. Exciton binding energy (in unit R_{\perp}) as a function of anisotropy parameter $\alpha\beta$.

$(\alpha\beta)^{1/3}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
This work	3.229 99	2.713 59	2.321 40	2.011 58	1.760 39	1.553 03	1.379 56	1.232 86	1.107 67	1.000 00
Ref. 13	...	2.694	2.321	2.0116	1.7604	1.553	1.3796	1.2329	1.1077	1.0000
Ref. 11	3.17	2.69	2.31	2.01	1.759	1.553	1.380	1.233	1.108	1.000
Ref. 10	3.123	2.667	2.300	2.002	1.756	1.551	1.379	1.233	1.108	1.000
$(\alpha\beta)^{-1/3}$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
This work	0.025 20	0.098 11	0.199 55	0.315 08	0.435 94	0.556 93	0.675 09	0.788 78	0.897 20	1.000 00
Ref. 13	...	0.0949	0.1992	0.3150	0.4358	0.5568	0.6750	0.7888	0.8972	1.0000
Ref. 10 ^a	0.0240	0.0962	0.1976	0.3135	0.4348	0.5562	0.6747	0.7886	0.8971	1.0000

^aCalculated with Ref. 10's method for $\alpha\beta > 1$.

where a central-five point formula is used for the second derivative.²⁶ To achieve an accuracy of $(10^{-4}-10^{-5})R_{\perp}$ for the eigenvalue of Eq. (7) in the range $0.2 \geq (\alpha\beta)^{1/3} \leq 5$, the maximum ℓ needed is $L_{\max}=20$, and the segment number is $N=60$ with an appropriately chosen scale factor k . For $(\alpha\beta)^{1/3}=0.1$ or 10, the maximum ℓ needed is 26. Smaller k is better for the case of stronger anisotropy, i.e., stronger localization, and the higher excited states prefer the use of larger k . For the $1s$ ground state, the exciton binding energy as a function of $\alpha\beta$ is listed in Table I, compared with the results of Refs. 10, 11, and 13. Our results are more accurate for the cases of strong anisotropy.

B. Magnetic field $B \neq 0$

The perturbative Hamiltonian due to the magnetic field can be written as

$$\delta H_B = \frac{\gamma^2}{4} (x^2 + y^2), \quad (8)$$

where the effective field $\gamma = \frac{1}{2}\hbar\omega_c/R_{\perp}$, and $\omega_c = eB/(c\mu_{\perp})$ is the in-plane cyclotron frequency. Since we are only interested in $m=0$ states, the term associated with the ordinary Zeeman effect has been ignored. The matrix elements to be added to Eq. (7) are

$$(\delta H_B)_{\ell\ell'} = \frac{\gamma^2}{4} r^2 \langle Y_{\ell'0} | \sin^2 \theta | Y_{\ell 0} \rangle. \quad (9)$$

For the isotropic exciton, Ref. 26 found that a value of $L_{\max}=12$ is adequate to give the four-digit accuracy for $\gamma \leq 5$. In our calculation, we find that a maximum ℓ of 20 can give an accuracy of $(10^{-4}-10^{-5})R_{\perp}$ for the ground state energy in a range of $0.2 \geq (\alpha\beta)^{1/3} \leq 5$ and $0 \geq \gamma \leq 10$. Only for the most extreme cases of $(\alpha\beta)^{1/3}=0.1$ or 10, a maximum ℓ of 26 is needed. For the $1s$ ground state, the shift of the energy level as a function of variables $\alpha\beta$ and γ is listed in Table II.

III. DISCUSSION AND APPLICATION

A. Binding energy of a simple anisotropic exciton

When the anisotropy is weak, $|(1-\alpha\beta)| \ll 1$, the eigenvalue of Eq. (7) can be obtained perturbatively by using the

wave-function of an isotropic exciton. A series expansion was given by Wheeler and Dimmock.⁷ Here, we give a closed form as:

$$E = 1 - \frac{2 \arcsin \sqrt{1-\alpha\beta}}{\sqrt{1-\alpha\beta}} = - \left(1 + \frac{1-\alpha\beta}{3} + \frac{3(1-\alpha\beta)^2}{20} + \frac{5(1-\alpha\beta)^3}{56} + O[(1-\alpha\beta)^4] \right). \quad (10)$$

A slightly different approximation was used by Hopfield and Thomas:⁶ introducing an averaged reduced mass

$$\frac{1}{\mu_0} = \frac{1}{3} \left(\frac{2}{\mu_{\perp}} + \frac{1}{\mu_{\parallel}} \frac{\epsilon_{\perp}}{\epsilon_{\parallel}} \right),$$

and rewriting Eq. (1) by substituting for μ_0 , the first order perturbation yields

$$E = -\frac{3}{2+\alpha\beta} = - \left(1 + \frac{1-\alpha\beta}{3} + \frac{(1-\alpha\beta)^2}{9} + \frac{(1-\alpha\beta)^3}{27} + O[(1-\alpha\beta)^4] \right). \quad (11)$$

Equations (10) and (11) explain why $(\alpha\beta)^{1/3}$ was found to be a good parameter to describe the anisotropy effect on the binding energy by Faulkner.¹¹ In fact, simply taking $(\alpha\beta)^{-1/3}$ as the binding energy, the result is similar to Eqs. (10) and (11):

$$E = -\frac{1}{(\alpha\beta)^{1/3}} = - \left(1 + \frac{1-\alpha\beta}{3} + \frac{2(1-\alpha\beta)^2}{9} + \frac{14(1-\alpha\beta)^3}{81} + O[(1-\alpha\beta)^4] \right). \quad (12)$$

While Eqs. (10) and (11) underestimate the binding energy, for instance, by less than 2% and 4%, respectively, for $\alpha\beta = 0.5$, Eq. (12) overestimates the binding energy by less than 2%. The anisotropy in materials like CdS, CdSe, and partially ordered GaInP₂ are usually weaker than $\alpha\beta = 0.5$.

On the other hand, the variational method proposed by Kittel and Mitchell,⁹ Kohn and Luttinger,¹⁰ and Faulkner¹¹ can cover a much larger range of anisotropy. Even for

TABLE II. (a) Energy shift (in unit R_0) of the exciton ground state as a function of effective magnetic field γ for anisotropy parameter $\alpha\beta < 1$.

$(\alpha\beta)^{1/3}$										
γ	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.05	0.000 29	0.000 36	0.000 44	0.000 52	0.000 62	0.000 72	0.000 84	0.000 96	0.001 10	0.001 25
0.1	0.001 18	0.001 45	0.001 75	0.002 09	0.002 47	0.002 88	0.003 34	0.003 83	0.004 37	0.004 95
0.2	0.004 70	0.005 78	0.006 98	0.008 32	0.009 79	0.011 40	0.013 16	0.015 05	0.017 08	0.019 24
0.3	0.010 54	0.012 93	0.015 59	0.018 52	0.021 74	0.025 23	0.028 98	0.032 97	0.037 20	0.041 63
0.4	0.018 65	0.022 81	0.027 43	0.032 50	0.037 99	0.043 89	0.050 16	0.056 77	0.063 66	0.070 79
0.5	0.028 95	0.035 33	0.042 36	0.049 99	0.058 20	0.066 93	0.076 10	0.085 65	0.095 50	0.105 58
0.6	0.041 38	0.050 36	0.060 17	0.070 75	0.082 02	0.093 88	0.106 22	0.118 94	0.131 92	0.145 07
0.7	0.055 86	0.067 77	0.080 70	0.094 52	0.109 11	0.124 33	0.140 02	0.156 05	0.172 27	0.188 55
0.8	0.072 30	0.087 45	0.103 76	0.121 07	0.139 18	0.157 92	0.177 09	0.196 50	0.216 00	0.235 43
0.9	0.090 61	0.109 25	0.129 19	0.150 17	0.171 96	0.194 33	0.217 05	0.239 90	0.262 69	0.285 26
1.0	0.110 72	0.133 08	0.156 82	0.181 62	0.207 21	0.233 30	0.259 61	0.285 91	0.311 98	0.337 66
1.1	0.132 53	0.158 79	0.186 50	0.215 25	0.244 72	0.274 58	0.304 51	0.334 25	0.363 58	0.392 33
1.2	0.155 97	0.186 31	0.218 10	0.250 90	0.284 31	0.317 96	0.351 51	0.384 69	0.417 25	0.449 02
1.3	0.180 96	0.215 51	0.251 51	0.288 41	0.325 80	0.363 26	0.400 43	0.437 02	0.472 77	0.507 53
1.4	0.207 43	0.246 31	0.286 59	0.327 67	0.369 06	0.410 34	0.451 11	0.491 07	0.529 98	0.567 66
1.5	0.235 31	0.278 63	0.323 26	0.368 54	0.413 96	0.459 04	0.503 39	0.546 69	0.588 71	0.629 28
1.6	0.264 54	0.312 37	0.361 41	0.410 93	0.460 37	0.509 25	0.557 15	0.603 76	0.648 85	0.692 25
1.7	0.295 05	0.347 47	0.400 96	0.454 73	0.508 20	0.560 85	0.612 28	0.662 16	0.710 27	0.756 45
1.8	0.326 78	0.383 85	0.441 82	0.499 86	0.557 35	0.613 76	0.668 68	0.721 79	0.772 87	0.821 80
1.9	0.359 69	0.421 46	0.483 94	0.546 24	0.607 73	0.667 88	0.726 26	0.782 55	0.836 57	0.888 19
2.0	0.393 71	0.460 23	0.527 23	0.593 80	0.659 28	0.723 14	0.784 93	0.844 39	0.901 30	0.955 57
2.2	0.464 9	0.541 03	0.617 12	0.692 20	0.765 60	0.836 78	0.905 32	0.970 96	1.033 53	1.092 97
2.4	0.540 1	0.625 86	0.711 04	0.794 59	0.875 82	0.954 21	1.029 35	1.101 02	1.169 10	1.233 55
2.6	0.618 9	0.714 37	0.808 63	0.900 58	0.989 54	1.075 01	1.156 62	1.234 19	1.307 62	1.376 94
2.8	0.701 1	0.806 27	0.909 56	1.009 83	1.106 42	1.198 85	1.286 80	1.370 12	1.448 77	1.522 81
3.0	0.786 4	0.901 27	1.013 55	1.122 06	1.226 17	1.325 45	1.419 60	1.508 54	1.592 28	1.670 92
3.2	0.874 5	0.999 16	1.120 36	1.237 02	1.348 55	1.454 55	1.554 79	1.649 22	1.737 92	1.821 05
3.4	0.965 4	1.099 71	1.229 77	1.354 49	1.473 33	1.585 94	1.692 15	1.791 97	1.885 52	1.973 01
3.6	1.058 8	1.202 75	1.341 60	1.474 29	1.600 33	1.719 44	1.831 51	1.936 60	2.034 88	2.126 64
3.8	1.154 6	1.308 12	1.455 67	1.596 24	1.729 38	1.854 89	1.972 71	2.082 96	2.185 89	2.281 81
4.0	1.252 6	1.415 66	1.571 84	1.720 19	1.860 34	1.992 14	2.115 61	2.230 93	2.338 39	2.438 39
4.5	1.506 5	1.693 17	1.870 58	2.038 01	2.195 26	2.342 37	2.479 54	2.607 11	2.725 55	2.835 36
5.0	1.772	1.981 70	2.179 86	2.365 82	2.539 62	2.701 49	2.851 82	2.991 13	3.120 03	3.239 18
5.5	2.047	2.279 84	2.498 27	2.702 26	2.892 10	3.068 24	3.231 24	3.381 82	3.520 74	3.648 83
6.0	2.332	2.586 46	2.824 71	3.046 27	3.251 68	3.441 62	3.616 86	3.778 29	3.926 85	4.063 49
6.5	2.624	2.900 63	3.158 27	3.396 96	3.617 51	3.820 84	4.007 91	4.179 81	4.337 66	4.482 53
7.0	2.923	3.221 58	3.498 19	3.753 60	3.988 90	4.205 23	4.403 78	4.585 82	4.752 63	4.905 43
7.5	3.229	3.548 65	3.843 85	4.115 61	4.365 28	4.594 27	4.803 96	4.995 83	5.171 31	5.331 78
8.0	3.541	3.881 29	4.194 72	4.482 47	4.746 17	4.987 49	5.208 02	5.409 43	5.593 32	5.761 20
8.5	3.858	4.219 02	4.550 34	4.853 74	5.131 16	5.384 50	5.615 60	5.826 28	6.018 34	6.193 41
9.0	4.181	4.561 42	4.910 31	5.229 05	5.519 89	5.784 98	6.026 37	6.246 09	6.446 09	6.628 15
9.5	4.508	4.908 15	5.274 29	5.608 08	5.912 06	6.188 64	6.440 08	6.668 60	6.876 35	7.065 20
10.0	4.839	5.258 86	5.641 98	5.990 54	6.307 40	6.595 22	6.856 49	7.093 61	7.308 90	7.504 37

$(\alpha\beta)^{1/3}=0.2$ ($\alpha\beta=0.008$), their result only differs from Broeckx *et al.*,¹³ by 1% for the ground state. While the methods of Refs. 9, 10, and 11 give a similar accuracy, the former is much easier to use. Besides, we have now obtained analytical formulas for calculating the variational parameters in the former method. The trial function for Eq. (2) can be written as

$$f(x,y,z') = \sqrt{\frac{1}{\pi a^2 b}} \exp[-\sqrt{(x^2+y^2)/a^2+z'^2/b^2}]. \quad (13)$$

We find that with this trial function, the expectation value of the Hamiltonian in Eq. (12) can be given analytically, and the exciton ground state energy is

$$E = \min \left(\frac{2}{3a^2} + \frac{1}{3b^2} - \frac{2 \arctan \sqrt{\frac{a^2-b^2\alpha\beta}{b^2\alpha\beta}}}{\sqrt{a^2-b^2\alpha\beta}} \right). \quad (14)$$

The minimization conditions: $\partial E/\partial a=0$ and $\partial E/\partial b=0$ lead to the following equation for the parameter Q :

$$\sqrt{\frac{Q-\sqrt{\alpha\beta}}{\alpha\beta}} \frac{2+\sqrt{\alpha\beta}Q}{Q^2+2} = \arctan \sqrt{\frac{Q-\sqrt{\alpha\beta}}{\alpha\beta}}, \quad (15)$$

and the binding energy and parameters a and b are related to one of the two solutions of Eq. (15), Q_0 , which minimizes the energy:

TABLE II. (b) For $\alpha\beta > 1$.

γ	$(\alpha\beta)^{-1/3}$									
	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.05	0.03227	0.015 29	0.008 00	0.004 89	0.003 37	0.002 53	0.002 01	0.001 67	0.001 42	0.001 25
0.1	0.07619	0.045 54	0.027 60	0.018 12	0.012 92	0.009 85	0.007 89	0.006 57	0.005 64	0.004 95
0.2	0.169	0.1203	0.0841	0.0608	0.0460	0.0363	0.029 76	0.025 15	0.021 78	0.019 24
0.3	0.264	0.2030	0.1523	0.1163	0.0917	0.0740	0.062 33	0.053 43	0.046 76	0.041 63
0.4	0.361	0.2897	0.2268	0.1797	0.1457	0.1210	0.102 92	0.089 34	0.078 93	0.070 79
0.5	0.458	0.3787	0.3054	0.2482	0.2055	0.1737	0.149 65	0.131 27	0.116 94	0.105 58
0.6	0.556	0.4693	0.3868	0.3205	0.2697	0.2310	0.201 21	0.178 05	0.159 76	0.145 07
0.7	0.654	0.5611	0.4703	0.3957	0.3373	0.2920	0.256 67	0.228 83	0.206 57	0.188 55
0.8	0.753	0.6357	0.5554	0.4731	0.4076	0.3560	0.315 35	0.282 93	0.256 78	0.235 43
0.9	0.851	0.7471	0.6419	0.5523	0.4801	0.4226	0.376 75	0.339 88	0.309 90	0.285 26
1.0	0.950	0.8410	0.7294	0.6331	0.5545	0.4913	0.440 47	0.399 27	0.365 55	0.337 66
1.1	1.048	0.9354	0.8178	0.7152	0.6305	0.5619	0.506 20	0.460 79	0.423 41	0.392 33
1.2	1.147	1.0302	0.9070	0.7983	0.7079	0.6340	0.573 68	0.524 19	0.483 23	0.449 02
1.3	1.246	1.1254	0.9968	0.8824	0.7865	0.7075	0.642 72	0.589 25	0.544 80	0.507 53
1.4	1.345	1.2208	1.0872	0.9674	0.8661	0.7823	0.713 14	0.655 81	0.607 94	0.567 66
1.5	1.444	1.3165	1.1781	1.0531	0.9467	0.8582	0.784 81	0.723 70	0.672 50	0.629 28
1.6	1.543	1.4125	1.2695	1.1394	1.0282	0.9351	0.857 60	0.792 82	0.738 36	0.692 25
1.7	1.642	1.5086	1.3613	1.2264	1.1104	1.0129	0.931 41	0.863 05	0.805 40	0.756 45
1.8	1.742	1.6049	1.4534	1.3139	1.1933	1.0916	1.006 15	0.934 30	0.873 53	0.821 80
1.9	1.841	1.7014	1.5459	1.4019	1.2769	1.1710	1.081 75	1.006 48	0.942 65	0.888 19
2.0	1.940	1.7980	1.6386	1.4903	1.3611	1.2511	1.158 14	1.079 53	1.012 70	0.955 57
2.2	2.139	1.9917	1.8250	1.6684	1.5309	1.4132	1.313 06	1.227 98	1.155 33	1.092 97
2.4	2.338	2.1858	2.0122	1.8479	1.7026	1.5774	1.470 51	1.379 21	1.300 95	1.233 55
2.6	2.537	2.3803	2.2003	2.0287	1.8759	1.7437	1.630 18	1.532 89	1.449 22	1.376 94
2.8	2.736	2.5752	2.3891	2.2105	2.0506	1.9116	1.791 79	1.688 74	1.599 83	1.522 81
3.0	2.935	2.7704	2.5785	2.3932	2.2266	2.0810	1.955 15	1.846 52	1.752 53	1.670 92
3.2	3.134	2.9658	2.7684	2.5768	2.4037	2.2518	2.120 07	2.006 04	1.907 13	1.821 05
3.4	3.333	3.1615	2.9588	2.7611	2.5817	2.4238	2.286 40	2.167 13	2.063 44	1.973 01
3.6	3.532	3.3574	3.1496	2.9461	2.7607	2.5969	2.454 01	2.329 66	2.221 31	2.126 64
3.8	3.731	3.5535	3.3409	3.1317	2.9405	2.7711	2.622 79	2.493 50	2.380 61	2.281 81
4.0	3.931	3.7497	3.5325	3.3179	3.1211	2.9461	2.792 65	2.658 54	2.541 24	2.438 39
4.5	4.429	4.2410	4.0129	3.7855	3.5753	3.3873	3.221 46	3.075 82	2.947 92	2.835 36
5.0	4.928	4.7332	4.4950	4.2558	4.0332	3.8329	3.655 41	3.498 90	3.360 97	3.239 18
5.5	5.427	5.2260	4.9784	4.7282	4.4940	4.2822	4.093 70	3.926 88	3.779 41	3.648 83
6.0	5.927	5.7193	5.4631	5.2025	4.9573	4.7346	4.535 70	4.359 07	4.202 49	4.063 49
6.5	6.426	6.2132	5.9487	5.6784	5.4228	5.1898	4.980 92	4.794 91	4.629 61	4.482 53
7.0	6.925	6.7075	6.4353	6.1557	5.8902	5.6474	5.428 97	5.233 97	5.060 30	4.905 43
7.5	7.425	7.2022	6.9226	6.6342	6.3594	6.1071	5.879 53	5.675 89	5.494 16	5.331 78
8.0	7.924	7.6973	7.4105	7.1138	6.8300	6.5686	6.332 32	6.120 35	5.9309	5.761 20
8.5	8.424	8.1926	7.8991	7.5944	7.3019	7.0319	6.787 13	6.5671	6.3701	6.193 41
9.0	8.924	8.6882	8.3883	8.0759	7.7751	7.4967	7.243 75	7.0160	6.8117	6.628 15
9.5	9.424	9.1841	8.8779	8.5581	8.2494	7.9628	7.702 03	7.4667	7.2554	7.065 20
10.0	9.924	9.6802	9.3680	9.0411	8.7246	8.4303	8.161 83	7.9192	7.7011	7.504 37

$$E = -\frac{3Q_0(2 + \sqrt{\alpha\beta}Q_0)}{\sqrt{\alpha\beta}(Q_0^2 + 2)^2}, \quad (16)$$

$$\alpha = \frac{(\alpha\beta)^{1/4}(Q_0^2 + 2)}{3\sqrt{Q_0}}, \quad (17)$$

$$b = \frac{(Q_0^2 + 2)}{3Q_0}. \quad (18)$$

The other trivial solution of Eq. (15) is $Q = \sqrt{\alpha\beta}$ that does not minimize the energy. In fact, this solution leads to the approximation of Eq. (11).

Figure 1 compares the exciton binding energy as a function of $\alpha\beta$ according to Eqs. (10), (11), and (14). The result of Eq. (14) differs from that of the Eq. (7) (not shown in Fig. 1) by less than 0.5% for $\alpha\beta = 0.1$ or 10.

B. Diamagnetic shift of a simple anisotropic exciton

In the low-field region of $\gamma \ll 1$, the shift of the exciton state, defined as $\delta E = E(B) - E(B=0)$ (the so-called diamagnetic shift), can be evaluated perturbatively as $\delta E = \langle \Psi_0 | \delta H_B | \Psi_0 \rangle$, where Ψ_0 is the eigenstate of $B=0$.

Applying the approximation of Wheeler and Dimmock,⁷ the anisotropy only shifts the energy level, but has no effect on the diamagnetic shift, assuming the same values of μ_{\perp} and ϵ_0 . On the other hand, with the averaged-mass approximation of Hopfield and Thomas,⁶ the diamagnetic shift is

$$\delta E = \frac{\gamma^2}{2} \left(\frac{3}{2 + \alpha\beta} \right)^{-2}. \quad (19)$$

Equation (19) indicates that the diamagnetic shift becomes smaller (larger) if $\alpha\beta$ is smaller (larger) than 1, assuming μ_{\perp}

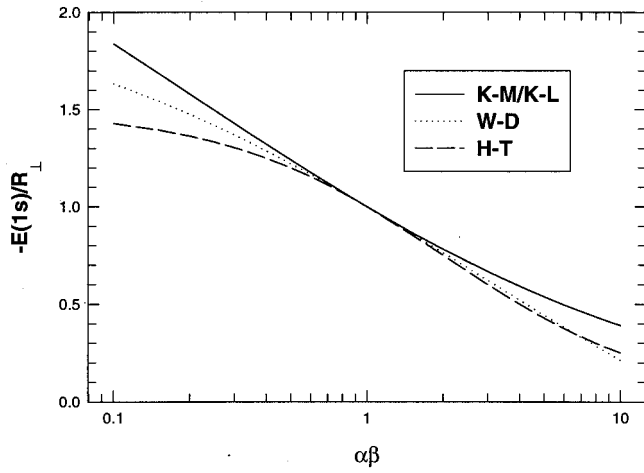


FIG. 1. Exciton binding energy as a function of anisotropy parameter $\alpha\beta$, evaluated by three approximations: *K-M/K-L* (Refs. 9 and 10), *W-D* (Ref. 7), and *H-T* (Ref. 6).

and ϵ_0 are kept the same. When $2|(1-\alpha\beta)/3| \ll 1$, the anisotropy has very little effect on the diamagnetic shift. While for the exciton binding energy, the approximation of Ref. 6, given by Eq. (11), is able to give a result with 4% accuracy for $\alpha\beta=0.5$; for the diamagnetic shift, Eq. (19) gives a larger error of 9% for $\gamma=0.1$.

When the anisotropy is not so weak, Lee and Lee¹⁶ recently proposed a way of calculating the magnetic shift by introducing an effective coupling constant for the Coulomb interaction. Let

$$e^{*4} = e^4 \min \left(-\frac{2}{3a^2} - \frac{1}{3b^2} + \frac{2 \arctan \sqrt{\frac{a^2 - b^2 \alpha\beta}{b^2 \alpha\beta}}}{\sqrt{a^2 - b^2 \alpha\beta}} \right), \quad (20)$$

then the anisotropic magnetoexciton is treated as an isotropic one with a reduced mass of μ_\perp and the effective Coulomb interaction e^{*2} . This approach may give rather accurate results when both the anisotropy and field are not too strong. For instance, for $\alpha\beta=0.5$ and $\gamma=1.0$, the error for δE is about 4% if the isotropic equation with an effective interaction is solved numerically. However, the variational approach used by the authors¹⁶ was less accurate (the error would be 12% for this case). Figure 2 shows a comparison for $\alpha\beta=0.1$ between the two approaches: directly solving the anisotropic magnetoexciton with the given anisotropy and solving the isotropic magnetoexciton with the effective interaction.

Notice that, because in the low-field region a dependence of $\delta E = c(\mu_\perp, \alpha\beta)B^2$ is always a good approximation (c is a constant), we can not deduce two parameters μ_\perp and $\alpha\beta$ independently by fitting experimental data to the theory, although $c(\mu_\perp, \alpha\beta)$ can be a complicated function of parameters μ_\perp and $\alpha\beta$. Nevertheless, it has been shown that in the low-field region by analyzing data including the excited states and/or with different field directions, one can indeed obtain the two parameters independently.^{6,7,17}

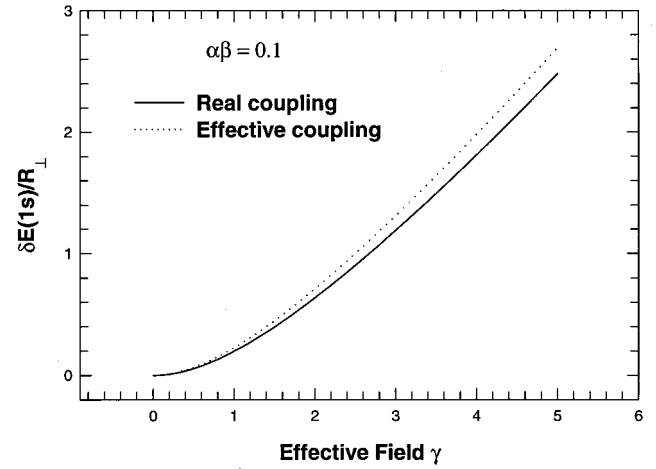


FIG. 2. A comparison of diamagnetic shift as a function of the field between two approaches: real coupling directly solving the anisotropic magnetoexciton with the given anisotropy and effective coupling solving the isotropic magnetoexciton with the effective interaction.

Also notice that in the high-field limit of the Landau-level region, the energy level is independent of the anisotropy parameter:

$$E = \left(n + \frac{1}{2} \right) \frac{e\hbar B}{\mu_\perp c}. \quad (21)$$

Thus, the experimental data in the intermediate field region is expected to be more useful for obtaining the two parameters μ_\perp and $\alpha\beta$ simultaneously. To illustrate this, Fig. 3 shows δE as a function of γ for three typical $\alpha\beta$ values, as well as the ratios of δE between $\alpha\beta=0.5$ and $\alpha\beta=1.0$ and between $\alpha\beta=0.1$ and $\alpha\beta=1.0$. As we can see, in the intermediate field region, the ratio has a relatively strong dependence on the field, which implies that the energy shift is more sensitive to the anisotropy parameter.

As an example, Fig. 4 shows a fitting of the experimental data to our numerical calculation for a partially ordered GaInP₂ sample. If the fitting is performed in the field region

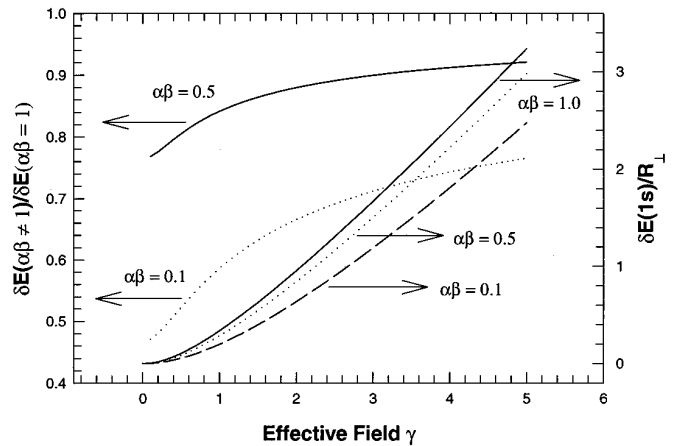


FIG. 3. Diamagnetic shift as a function of the field for anisotropy parameter $\alpha\beta=1.0, 0.5$, and 0.1 , and the ratio of the shift between $\alpha\beta=0.5$ and 0.1 to $\alpha\beta=1.0$.

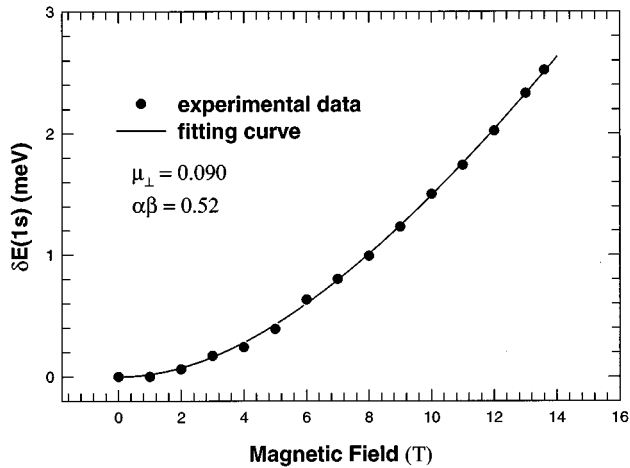


FIG. 4. Experimental and fitting results for an ordered GaInP₂ alloy.

$B \geq 6$ T, the yielded parameters are $\mu_{\perp} = 0.090 \pm 0.001$ and $\alpha\beta = 0.52 \pm 0.06$. These values agree well with the results obtained by fitting the experimental data of the low-field region ($B \leq 6$ T) in two field directions to perturbative formulas:¹⁷ $\mu_{\perp} = 0.0915 \pm 0.0005$ and $\alpha\beta = 0.61 \pm 0.16$. The error bar for $\alpha\beta$ is relatively large, which is because of the fact that it is a less sensitive parameter in determining the exciton level.

IV. CONCLUSION

We have applied a numerical technique to calculate eigenstates of an anisotropic magnetoexciton. Numerical results are tabulated for the range of $0.1 < \alpha\beta^{1/3} < 10$ and $0 \leq \gamma \leq 10$, which can be directly used for fitting experimental data to obtain the in-plane exciton reduced mass and the anisotropic parameter $\alpha\beta$. Various approximations are discussed and compared in terms of their applicable regions. We have demonstrated that by only measuring and analyzing the magnetic shift of the exciton ground state with the field aligned in the uniaxis, both the in-plane reduced mass and the anisotropic parameters can be obtained.

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- ¹G. Dresselhaus, Phys. Rev. **106**, 76 (1957).
- ²M. Altarelli and N. O. Lipari, Phys. Rev. B **9**, 1733 (1974).
- ³L. Swierkowski, Phys. Rev. B **10**, 3311 (1974).
- ⁴K. Cho, S. Suga, W. Dreybrodt, and F. Willmann, Phys. Rev. B **11**, 1512 (1975).
- ⁵N. O. Lipari and M. Altarelli, Solid State Commun. **33**, 47 (1980).
- ⁶J. J. Hopfield and D. G. Thomas, Phys. Rev. **122**, 35 (1961).
- ⁷R. G. Wheeler and J. O. Dimmock, Phys. Rev. **15**, 1805 (1961).
- ⁸R. L. Greene and K. K. Bajaj, Phys. Rev. B **31**, 6498 (1985).
- ⁹C. Kittel and A. H. Mitchell, Phys. Rev. **96**, 1488 (1954).
- ¹⁰W. Kohn and J. M. Luttinger, Phys. Rev. **98**, 915 (1955).
- ¹¹R. A. Faulkner, Phys. Rev. **184**, 713 (1969).
- ¹²A. Baldereschi and M. G. Diaz, Nuovo Cimento B **68**, 217 (1970).
- ¹³J. Broeckx, P. Clauws, and J. Vennik, J. Phys. C:Solid State Phys. **19**, 511 (1986).
- ¹⁴C. M. Dai, J. H. Pei, and D. S. Chuu, Physica B **160**, 317 (1990).
- ¹⁵A. Twardowski and J. Jinter, Phys. Status Solidi B **110**, 47 (1982).
- ¹⁶K.-S. Lee and E. Lee, J. Korean Phys. Soc. **29**, 824 (1996).
- ¹⁷P. Ernst, Y. Zhang, F. A. J. M. Driessen, A. Mascarenhas, E. D. Jones, C. Geng, F. Scholz, and H. Schweizer, J. Appl. Phys. **81**, 2814 (1997).
- ¹⁸Y. Zhang and A. Mascarenhas, Phys. Rev. B **51**, 13 162 (1995).
- ¹⁹Y. Yafet, R. W. Keyes, and E. N. Adams, J. Phys. Chem. Solids **1**, 137 (1956).
- ²⁰D. M. Larsen, J. Phys. Chem. Solids **29**, 271 (1968).
- ²¹E. P. Pokatilov and M. M. Rusanov, Sov. Phys. Solid State **10**, 2458 (1969).
- ²²B. Gerlach, D. Richter, and J. Pollmann, Z. Phys. B **66**, 419 (1987).
- ²³H. Ruder, G. Wunner, H. Herold, and M. Reinecke, J. Phys. B:At. Mol. Phys. **14**, L45 (1981).
- ²⁴V. B. Pavlov-Verevkin and B. I. Zhilinskii, Phys. Lett. **75A**, 279 (1980).
- ²⁵M. Cohen and G. Herman, J. Phys. B:At. Mol. Phys. **14**, 2761 (1981).
- ²⁶D. Cabib, E. Fabri, and G. Fiorio, Solid State Commun. **9**, 1517 (1971); Nuovo Cimento B **10**, 185 (1972).
- ²⁷C. Aldrich and R. L. Greene, Phys. Status Solidi B **93**, 343 (1979).
- ²⁸P. C. Makado and N. C. McGill, J. Phys. C:Solid State Phys. **19**, 873 (1986).
- ²⁹F. Bassani and G. P. Parravicini, *Electronic States and Optical Transitions in Solids* (Pergamon, Oxford, 1975), p. 188.