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A full numerical calculation of the Franz–Keldysh effect on magnetoexcitons in a bulk semiconductor*

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We have performed a full numerical calculation of the Franz–Keldysh (FK) effect on magnetoexcitons in a bulk GaAs semiconductor. By employing an initial value method in combination with the application of a perfect matched layer, the numerical effort and storage size are dramatically reduced due to a significant reduction in both computed domain and number of base functions. In the absence of an electric field, the higher magnetoexcitonic peaks show distinct Fano lineshape due to the degeneracy with continuum states of the lower Landau levels. The magnetoexcitons that belong to the zeroth Landau level remain in bound states and lead to Lorentzian lineshape, because they are not degenerated with continuum states. In the presence of an electric field, the FK effect on each magnetoexcitonic resonance can be identified for high magnetic fields. However, for low magnetic fields, the FK oscillations dominate the spectrum structure in the vicinity of the bandgap edge and the magnetoexcitonic resonances dominate the spectrum structure of higher energies. In the moderate electric fields, the interplay of FK effect and magnetoexcitonic resonance leads to a complex and rich structure in the absorption spectrum.

Keywords: Franz–Keldysh effect, magnetoexciton, bulk semiconductor, optical absorption spectrum
PACC: 7820J, 7820L, 7820B

1. Introduction

The optical properties of semiconductors have been extensively investigated for decades because of their wide applications in optoelectronic and photonic devices. The geometric confinements and external fields can further modify the optical properties of semiconductors significantly. Application of an external electric field leads to a modulation of the optical absorption spectrum near the band edge, which is known as the Franz–Keldysh (FK) effect.[1,2] The modulation is nonperiodic and scaled with $|F|^{2/3}$ and the absorption is nonzero and decreases exponentially below the gap, which follows the asymptotics of the Airy function and is a consequence of the unbounded energy spectrum for the electrons and the holes. Meanwhile, an external magnetic field can drastically change the optical absorption spectrum further.[3−5] The application of a magnetic field to a bulk semiconductor results in a series of Fano resonances arising from the quantum interference between high lying excitonic states and lower-energy continua.[6,7] However, to model the electro-optic and magneto-optic properties of a semiconductor at low temperatures accurately, one must also include the excitonic effects, which is a bound state of a electron and a hole by attractive Coulomb interaction between them.[8,9] The effects of electric fields on excitonic absorption in quantum wells have been widely used as an electro-optical modulator in modern optical communication, since the excitonic effects in quantum-well structures are much more pronounced and can be observed clearly even at room temperature.[10−12] The mechanism behind these enhanced excitonic effects is the so-called quantum-confined Stark effect.[13,14]

The optical properties in low-dimensional semiconductor structures are an active research topic in semiconductor physics. Reviews about the methods of calculating the optical susceptibility of low-dimensional semiconductors have been presented in recently published books.[15,16] Analytical formulae of the excitonic optical absorption of three-

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dimensional (3D), two-dimensional, one-dimensional, and d-dimensional with $d \in(1,\infty)$ semiconductors have been derived. However, analytical solutions are available only for a few idealized and simplified models, which are not of particular interest, thus it is vital to have an efficient numerical method to calculate the optical absorption. Though a large number of numerical calculations have been performed for low-dimensional semiconductor structures,[17−29] there are only very few reports on the full numerical simulation of optical absorption in a bulk semiconductor.[6,7,16,30] This is partially due to the huge storage memory and numerical effort required for full numerical 3D bulk simulations. In this paper, we use an efficient method to investigate the FK effect on the magnetoexcitonic absorption in a 3D bulk semiconductor. The method is based upon the discretization of the Hamiltonian in real space and the solution of the initial-value problem in real time.[16,31] Liu and Zhu have applied this initial-value problem method to simulating the optical absorption in a superlattice under a terahertz field.[32] Similar methods have also been used to solve optical absorption in terahertz-field-driven quantum wells,[33,34] nanorings,[35,36] quantum wires,[37] and quantum dot superlattice in a nanowire or nanoring,[22,38] recently. The FK effects on Landau levels and magnetoexcitons in quantum wells were investigated by Citrin and Hughens.[39] However, to the best of our knowledge, this is the first full numerical calculation of the FK effect on the magnetoexcitons in a 3D bulk semiconductor.

2. Formulation and numerical method

2.1. Formulation of the initial-value problem

The linear optical properties of a semiconductor are characterized by the linear optical susceptibility, $\chi(t,t')$, which relates the optical field $E(t)$ with the polarization $P(t)$ induced by $E(t)$ via

$$P(t)=\int_{-\infty}^{t}\mathrm{d}t'\epsilon_0\chi(t,t')E(t'), \tag{1}$$

where ϵ_0 is the dielectric constant of vacuum. By performing Fourier transform, one obtains the definition of linear optical susceptibility in the frequency domain,

$$\chi(\omega)=\frac{\tilde{P}(\omega)}{\epsilon_0\tilde{E}(\omega)}. \tag{2}$$

The macroscopic polarization in a semiconductor is related to the electron–hole-pair amplitude $\psi(\boldsymbol{r}_\mathrm{e},\boldsymbol{r}_\mathrm{h},t)$ by

$$P(t)=\frac{1}{\Omega}d^*\int\mathrm{d}^3\boldsymbol{r}\psi(\boldsymbol{r},\boldsymbol{r},t), \tag{3}$$

where Ω is the normalization volume, and d^* is the complex conjugate of the dipole matrix element d.

The optical susceptibility can be obtained by using several approaches, such as eigenvalue problem,[40] boundary-value problem,[41] and initial-value problem.[31] A comparison between these different methods has been done in Ref.[16]. It is because of the advantage of efficient storage and numerical solving that we make use of the initial-value problem method in this paper. To determine the electron–hole-pair amplitude, one solves the time-dependent inhomogeneous Schrödinger equation

$$\mathrm{i}\hbar\frac{\mathrm{d}\psi(t)}{\mathrm{d}t}=\hat{H}\psi(t)-\mathrm{i}\hbar\gamma\psi(t)-\mathrm{d}\delta(\boldsymbol{r}_\mathrm{e}-\boldsymbol{r}_\mathrm{h})E(t), \tag{4}$$

where $\hat{H}$ is the Hamiltonian of the system considered, $\hbar$ is Planck's constant, and γ is a phenomenological dephasing constant. We investigate the FK effect on magnetoexcitons of a bulk semiconductor in the Faraday configuration, in which the directions of the electric field and the magnetic field are coincident. In this configuration, the Hamiltonian of a bulk magnetoexciton under an electric field is given by

$$\begin{aligned}\hat{H}=&-\frac{1}{2m_\perp}\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right)-\frac{1}{2m_{//}}\frac{\partial^2}{\partial z^2}\\&-\frac{e^2}{4\pi\epsilon_0\epsilon\sqrt{\rho^2+z^2}}+eFz\\&+\frac{1}{8m_\perp}e^2B^2\rho^2,\end{aligned} \tag{5}$$

where $m_\perp$ and ρ are the reduced mass and the relative distance between the electron and the hole in the plane perpendicular to the direction of the electric and magnetic fields, respectively; $m_{//}$ and z are the reduced mass and the relative distance along the direction of the electric and magnetic fields, respectively; e is the elementary charge, F is the electric field, and B is the magnetic field. The first term on the right-hand side of Eq.(5) describes the kinetic energy in the plane perpendicular to the field direction, the second term describes the kinetic energy along the field direction, the third term describes the Coulomb interaction between the electron and the hole, the fourth term describes the effects of an external electric field, and the last term describes the effects of an external magnetic field.

2.2. Perfect matched layer technique

A major progress in solving the wave equations of electromagnetism and quantum mechanics in real space is the introduction of absorbing boundary conditions, which leads to a significant reduction in both memory and numerical effort. The purpose of introducing the absorbing boundary conditions is to simulate the wave propagation in an infinite domain by suppressing the reflection of the wavepackets at the artificial boundaries. Various absorbing boundary conditions have been proposed for electromagnetic wave calculations.[42−45] A perfect matched layer (PML) technique has been widely used in electromagnetic finite difference time domain simulation due to its effectiveness and convenience.[45,46] The idea of absorbing boundary conditions in quantum mechanics calculation is to modify the Hamiltonian to suppress the reflection of waves at boundary of the finite calculation domain. Ahland *et al*[47] have used a PML technique and demonstrated the usefulness of PML for the calculation of the optical absorption in the presence of continuum states. The PML is realized by the introduction of complex stretched coordinates. Latterly, Glutsch *et al*[48] also demonstrated the PML by using complex effective mass in the artificial absorbing layers, and they could calculate the optical absorption of a superlattice in the regime of the Zener breakdown. And very recently, the PML was used to treat the superlattice in the Voigt geometry.[49] Candidates for absorbing boundary conditions are suggested for those directions, where (i) the initial wavepacket is localized near the origin, (ii) the polarization is of interest only in a small region around the origin, and (iii) the potential approaches a constant far from the origin so that the time evolution of polarization is the same as for a free particle.[16] In this paper, we use the complex effective mass formulation. Thus, the Hamiltonian of kinetic energy along the field direction, z axis, becomes

$$\hat{H}_{\parallel} = -\frac{\partial}{\partial z}\frac{1}{2m_{\parallel}(z)}\frac{\partial}{\partial z}. \tag{6}$$

This expression is the typical form of a Hamiltonian when the mass of particle depends on coordinate. But, in this case, the coordinate-dependent mass is complex. The mass is chosen as

$$\begin{aligned} &m_{\parallel}(z) = 1 \quad \text{for} \quad |z| \le \frac{L_1}{2}; \\ &m_{\parallel}(x) \to |\infty| \mathrm{e}^{\mathrm{i}\alpha} \quad \text{for} \quad z \to \pm\frac{L_2}{2}; \quad 0 < \alpha < \pi, \end{aligned} \tag{7}$$

where L_1 and L_2 is the boundary of the PML and the computed domain, respectively. The usefulness of the complex effective mass is twofold: an increase in real part reduces the wavelength for a fixed energy and the imaginary part leads to the damping of the wave packet.

3. Numerical results and discussion

To simplify the calculations, we use excitonic Hartree units in this paper. The major advantage is that all quantities will be in the order of unity in the numerical calculation.[16] The units for energy, length, time, electric field, and magnetic field, for GaAs parameters, are $[E]$ = 9.37 meV, $[a]$ = 11.7 nm, $[t]$ = 70.3 fs, $[F]$ = 7.98 kV/cm, and $[B]$ = 4.78 T, respectively. Since the motion in the plane perpendicular to the electric and magnetic field is confined by the magnetic field, the computed domain in this plane can be reduced, because the extension of the wavefunction can be estimated by the classical return point. Thus, the PML need not be applied to the radial direction. However, special attention must be paid to the direction along the electric field and the magnetic field. The numerical solution tends to be divergent since the quantity eFz will be very large if the size of the domain is large. It is suggested that the PML be applied to the direction where the potential approaches a constant far from the origin as mentioned in the last section. However, to avoid these divergences, we apply the PML to the electric field direction and modify the static electric potential in the PML from liner to constant. By this modification, we can reduce significantly the computed domain and remove the divergence. From our experience, the results obtained by applying the PML are hardly discernible from those obtained without the use of the PML but in a very large computation domain.

To demonstrate the validity of our approach, we show the FK effect of the optical absorption in a bulk semiconductor under an electric field. In Fig.1, we show the absorption spectrum of a bulk GaAs under different electric fields with field strengths F =0, 0.25, 0.5, 1.0 and 2.0. In this and the following figures, the zero of the energy scale is the gap energy at zero temperature. The spectrum consists of a Rydberg series of s excitons below the bandgap edge and a continuum above the bandgap edge. But for any $F \neq 0$,

the spectrum becomes entirely continuous. The FK oscillations resulting from the oscillating behaviour of the Airy function show up above the bandgap edge. The spectrum extends into the bandgap due to the unbounded energy spectrum for the electrons and the holes. The decrease is exponential resulting from the asymptotics of the Airy function. The inset is the enlarged part of the spectrum near the bandgap edge to show the details. The present results already had been obtained for a bulk semiconductor in an electric field decades ago by an approximate analytical or a semi-numerical solution,[50] and is in good agreement with the results obtained with no boundary conditions existing (i.e. without PML). However, our approach leads to a reduction in memory by about a factor of 10 by employing the PML techniques.

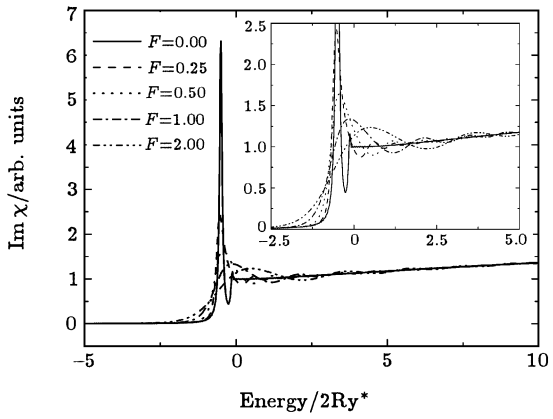


Fig.1. Optical absorption versus energy for a bulk semiconductor under different electric fields. The field strength is $F = 0$ (solid line), $F = 0.25$ (dashed line), $F = 0.5$ (dotted line), $F = 1.0$ (dash-dotted line), and $F = 2.0$ (dash-dot-dotted line), respectively. The inset is the enlarged part of the spectrum near the bandgap edge to show the details of the FK effect. The spectrum has FK oscillations appearing above the bandgap edge and extends to the bandgap for $F \neq 0$. For $F = 0$, The spectrum consists of a series of s excitons below the bandgap edge and a continuum above the bandgap edge.

Figure 2 shows the absorption spectrum of a GaAs bulk semiconductor under different magnetic fields with the field strengths B =0, 0.25, 0.5, 1.0, 2.0 and 4.0, respectively. The successive traces are offset vertically for clarity. Below the continuum onset, there are a series of discrete lines. Only the 1s exciton is resolved because of the finite homogeneous broadening. The magnetoexcitons belonging to the zeroth Landau level show Lorentzian lineshape. The binding energy of the lowest exciton increases compared with the case of no magnetic field. For small magnetic fields, the absorption resembles the one without magnetic fields, except for a small modulation of nearly equidistant peaks appearing. And the modulation stems from the Landau quantization of the orbits in the plane perpendicular to the magnetic field. The lineshapes of these resonances cannot be clearly identified. With the increase of magnetic field, clear and distinct Fano resonances emerge. This is because the higher Landau levels are degenerated with the continuum states of the lower Landau levels. But the magnetoexcitons belonging to the zeroth Landau level show Lorentzian lineshape because there does not exist the continuum of lower energy states. For a fixed Landau index, the heights of the Fano resonance peaks increase about linearly with the magnetic field. The spacing between the resonances is also linear in field. In contrast to the Fano resonance peaks, the shift of the ground state is quadratic in the field. In the high-field limit, the Fano–Rydberg series of different Landau levels are well separated by continua, for which the absorption is nearly constant. The energetic spacing between

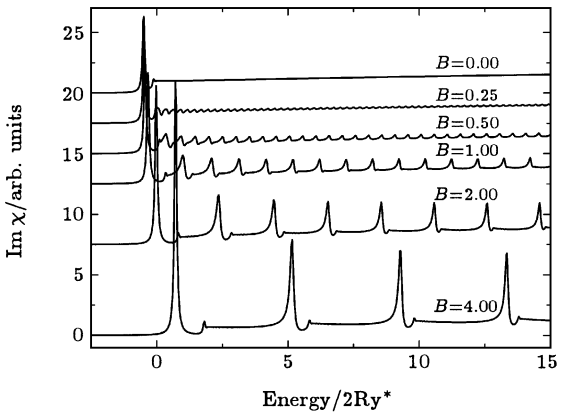


Fig.2. Optical absorption versus energy for a bulk semiconductor under different magnetic fields. The field strength is $B = 0$, $B = 0.25$, $B = 0.5$, $B = 1.0$, $B = 2.0$, and $B = 4.0$, separately. For low magnetic fields, the spectrum resembles the continuum of the spectrum without magnetic field ($B = 0$) except for small modulation of resonant peaks appearing due to Landau quantization. The lineshapes of these resonant peaks cannot be clearly identified. For high magnetic fields, the spectrum consists of a series of distinct Fano resonant peaks separated by constant continuum. The resonant peaks increase with magnetic field increasing. And the lowest exciton has a blue-shift due to the diamagnetic shift.

the Landau levels, which is equal to the cyclotron frequency, is much larger than the natural linewidth. The ratio between the oscillator strengths of the 1s

exciton and the continuum has drastically increased. These Fano resonances in the optical absorption of bulk semiconductors under a magnetic field were obtained firstly by Glutsch *et al*,[6] and experimentally demonstrated.[7] But in Glutsch's original calculation, PML techniques were not employed. The PML leads to a reduction in computing time by about a factor of 6 in our calculation.

Having demonstrated the validity of the method, now we show the optical absorption spectrum of a bulk GaAs semiconductor in the presence of both an electric field and a magnetic field in the Faraday configuration. It is well known that the electronic states of magnetoexcitons are difficult to calculate accurately. The application of an electric field makes the problem even harder. As analytical solution is not available for

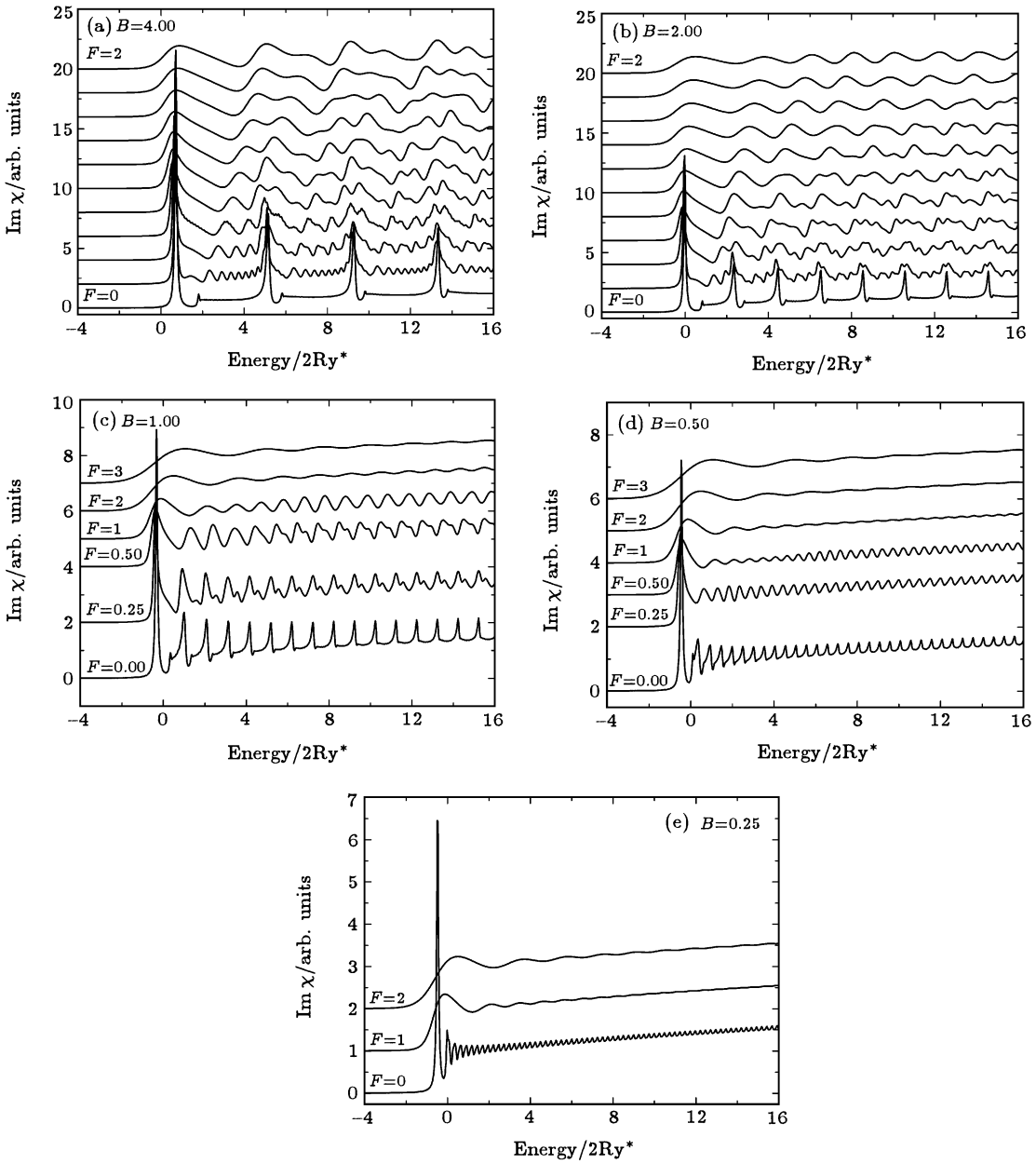


Fig.3. The FK effect of magnetoexcitons at different values of magnetic field $B = 4.0$ (a), $B = 2.0$ (b), $B = 1.0$ (c), $B = 0.5$ (d), and $B = 0.25$ (e), respectively. For high magnetic fields, as shown in (a) and (b), the continua between magnetoexcitons of different Landau level indices become modulated by FK oscillations and the absorption edges of the magnetoexcitons extend to the lower energy side. For low magnetic fields, as shown in (d) and (e), the FK effect dominates the spectrum structure in the vicinity of the bandgap edge, and the magnetoexcitonic resonances dominate the spectrum structure of higher energy. For the intermediate magnetic fields, as shown in (c), both situations of high magnetic fields and low magnetic fields show up with the strength of electric field increasing from low to high.

this complicated problem, it is vital to have an efficient numerical method to calculate the optical absorption in this configuration. The method presented in this paper is very flexible and efficient, we can make our calculations on this configuration without any additional complexity. To the best of our knowledge, this is the first report for a full numerical calculation on the FK effect on the magnetoexcitons in a bulk semiconductor. Figure 3 shows the effect of an electric field on the magnetoexcitonic optical absorption spectrum under different values of the magnetic field. Under high magnetic fields as shown in Fig.3(a) and Fig.3(b) for B=4.0 and B=2.0 respectively, the continua between magnetoexcitons of different Landau level indices become modulated by FK oscillations. The FK oscillations emerge above each magnetoexciton, and the absorption edges of the magnetoexcitons extend to the lower energy side. With the electric field increasing, the absorption spectrum transits from the resonances of Landau levels to FK resonances. In the region of a moderate field, the interplay of magnetoexcitonic resonances and FK oscillations results in complex and rich spectrum structures. Under low magnetic fields, as shown in Fig.3(d) and Fig.3(e) for B=0.5 and B=0.25 respectively, the FK effect dominates the spectrum structure in the vicinity of the bandgap edge, and the magnetoexcitonic resonances dominate the spectrum structures of higher energy above band edge. And with electric field increasing, the effect of magnetic field is quenched leaving only the effect of the electric field. For the intermediate magnetic field B=1 as shown in Fig.3(c), effects occurring in both situations of high magnetic fields and low magnetic fields show up with the strength of electric field increasing from low to high.

4. Conclusions

We have performed a full numerical calculation of the FK effect on magnetoexcitons in a bulk GaAs semiconductor. By the employing of an initial value method in combination with the application of PML, the numerical effort and storage size are drastically reduced due to a significant reduction in computed domain and number of base functions. In the absence of the electric field, the higher magnetoexcitonic peaks show distinct Fano lineshapes because of the degeneracy with continuum states of the lower Landau levels. The magnetoexcitons belonging to the zeroth Landau level remain in bound states and the corresponding peaks show up Lorentzian lineshapes, because they are not degenerated with continuum states. However, in the presence of the electric field, the optical absorption spectrum shows a series of complex and pronounced features due to the interplay of the FK oscillations and magnetoexcitonic resonances. If the electric field is not too high, the FK effect for each magnetoexcitonic resonance can be identified for high magnetic fields. For low magnetic fields, the electric field dominates the spectrum structure in the vicinity of the bandgap edge and the magnetoexcitonic resonances dominate the spectrum structure of higher energies. In the moderate electric fields, the interplay of FK effect and magnetoexcitonic resonance results in a complex structure in the absorption spectrum.

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