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Research Article

ENERGIES AND DIAMAGNETIC COEFFICIENTS OF EXCITON IN MONOLAYER WSe_2

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ABSTRACT

Two-dimensional exciton under a uniform magnetic field in monolayer transition-metal dichalcogenides (TMDCs) has been a fascinating problem for experimental and theoretical studies in the last decade due to its practical applications in electronic and optics devices. Specifically, there is significant interest in the diamagnetic coefficients of excitons in monolayer TMDCs, focusing on the monolayer WSe_2 encapsulated by boron nitride (h-BN). The discrepancy between theoretical calculations and experimental data for the diamagnetic coefficient of an exciton in monolayer TMDCs requires further improvement in theory for this material property. This paper uses the so-called modulated perturbation method by combining the Rayleigh-Schrödinger perturbation theory with the Levi-Civita transformation and including a variational parameter. The advantage of the constructed method is demonstrated in calculating the exciton diamagnetic coefficient within the second order of approximation. The results are then compared with recent experimental ones.

Keywords: diamagnetic coefficient; exciton; modulated perturbation method; TMDC

1. Introduction

Two-dimensional exciton in TMDCs is a typical problem that has been much researched since 2010, after the success of creating two-dimensional materials. Exciton is a quasiparticle created by electronic interactions between the hole and the electron, often described by the Keldysh potential (Keldysh, 1979). When an exciton exists under a magnetic field, it is also called magnetoexciton. The interest in magnetoexciton in TMDCs arises due to their band gap covering the near-infrared and the entire visible range, leading to semiconductor properties different from graphene materials (Thambiratnam, 2020). Studying magnetoexciton in TMDCs can help to understand more about its properties, particularly the diamagnetic coefficient, which is related to the diamagnetic shift phenomena in magnetoexciton energy spectra and crucial for photo-electronic applications.

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There have been several theoretical and experimental studies for calculating the diamagnetic coefficient of magnetoexciton in TMDCs, particularly in the monolayer WSe2 encapsulated by boron nitride (h-BN). However, experimental results are not in good agreement and cannot be truly interpreted by theoretical models. Specifically, the experiment by Stier et al. (2018) shows that beyond the 3s state, the diamagnetic coefficient cannot be yielded precisely from quadratic regression of magnetoexciton energies as predicted by the theory. Liu et al. (2019) showed that although their theoretical prediction model aligns with the experimental data from Stier et al. (2018), their experimental results for the diamagnetic coefficient were different. In the recent theoretical work by Ly et al. (2023), this discrepancy is attributed to the inaccuracy of the material parameters, such as exciton-reduced mass, the screening length, and the dielectric constant. This study then retrieves more accurate material parameters by analyzing the experimental data of Liu et al. (2019), compared to the exact numerical calculation. Using these retrieved material parameters, Ly et al. (2023) calculated the diamagnetic coefficients for WSe_2 and WS_2 by fitting the exact numerical energies with the perturbation term quadratically dependent on the magnetic field. However, based on our adjustment, the results could be more consistent if the theoretical energies used in the fitting procedure were from the second-order perturbation method.

On the other hand, it is well known that a two-dimensional magnetoexciton under the Levi-Civita transformation can be rendered to be an anharmonic oscillator model, which is a familiar system in condensed matter physics and thus easy to use various methods solving its Schrodinger equation (Hoang et al., 2013; Ly et al., 2022). *Particularly, the algebraic calculation by the FK operator method* (Feranchuk et al., 2015) *can be applied to this system.* In this study, we use the modulated perturbation method which combines the Rayleigh-Schrödinger perturbation theory with the Levi-Civita transformation and introduces a free parameter following the FK operator method to manipulate the rate of convergence of the perturbation theory schemes for numerical solutions. This modulated perturbation method allows us to calculate magnetoexciton energies for the ground and some low-lying excited states in the case of monolayer WSe_2. Furthermore, using the least mean square regression method, we can extract the diamagnetic coefficient of magnetoexciton from its energy spectra up to the second order of approximation and compare the results with the current studies.

2. Theoretical methods

2.1. The Schrödinger equation via the Levi-Civita transformation

First, we consider a neutral exciton that includes one electron and one hole interacting with each other by the potential $\hat{V}_{h-e}(r)$ in monolayer TMDCs. The movement of the exciton is constrained to the *xy* plane in the presence of a magnetic field $B\mathbf{e}_z$ perpendicular to the plane and along the z-axis. After separating the center-of-mass motion and assuming its momentum to be equal to zero at low temperatures, as in the most current experiments, the Schrödinger equation for relative motion is as follows:

$$\left\{\frac{1}{2\mu}\hat{\mathbf{p}}^2+\frac{1-\rho}{1+\rho}\frac{eB}{2\mu}\hat{l}_z+\frac{e^2B^2}{8\mu}r^2+\hat{V}_{h-e}(r)-E\right\}\psi(\mathbf{r})=0 \quad (1)$$

with the exciton reduced mass $\mu=m_e^*m_h^*/(m_e^*+m_h^*)$, the ratio of masses $\rho=m_e^*/m_h^*$, operators of the momentum $\hat{p}$, and angular momentum of the relative motion $\hat{l}_z$. The interaction between electron and hole $\hat{V}_{h-e}(r)$ is well described by the Keldysh potential expressed via the zero-order Struve and Bessel functions (Berkelbach, 2013; Keldysh, 1979). However, as shown in Ly et al. (2023), this potential can be rewritten in the Laplace form, which contains the average dielectric constant κ, the screening length r_0 related to the 2D polarizability χ_{2D} of the TMDC monolayer ($r_0=2\pi\chi_{2D}$).

Now, the Schrödinger equation in the *xy* space is written in the dimensionless form with the effective Hartree $E_H^*=\mu e^4/16\pi^2\varepsilon_0^2\hbar^2$, the Bohr effective radius $a_0^*=4\pi\varepsilon_0\hbar^2/\mu e^2$ for the energy and distance units, respectively, and the dimensionless magnetic field strength γ related to the magnetic field by the expression $B=\gamma\times\mu\hbar E_H^*/e$. After that, we take an important step to solve the equation using the Levi-Civita transformation (Levi-Civita, 1956): $x=u^2-v^2,\ y=2uv$ to convert equation (1) from *xy* space into *uv* space as

$$\left\{-\frac{1}{8}\left(\frac{\partial^2}{\partial u^2}+\frac{\partial^2}{\partial v^2}\right)+\left(\frac{1-\rho}{1+\rho}\frac{\gamma}{2}\hat{l}_z-E\right)\left(u^2+v^2\right)+\frac{\gamma^2}{8}\left(u^2+v^2\right)^3+\hat{V}_K(u,v)\right\}\psi(u,v)=0, \quad (2)$$

$$\hat{V}_K(u,v)=-\frac{1}{\kappa}\int_0^{+\infty}\frac{dq}{\sqrt{1+\alpha^2q^2}}\,(u^2+v^2)e^{-q\,(u^2+v^2)}. \quad (3)$$

Consequently, by employing the Levi-Civita transformation, the Hamiltonian can be rendered in a form similar to an anharmonic oscillator. This simple equation suggests the feasibility of using the algebraic calculation method, utilizing creation and annihilation operators (Feranchuk et al., 2015).

2.2. Algebraic calculation method

For the algebraic calculation, we introduce annihilation and creation operators $\hat{a},\ \hat{a}^+,\ \hat{b},\ \hat{b}^+$ as functions of $u,v,\partial/\partial u,\partial/\partial v$ with the definition details presented in Ly et al. (2023). These operators satisfy the conventional commutation relations

$$\left[\hat{a},\ \hat{a}^+\right]=1,\quad \left[\hat{b},\ \hat{b}^+\right]=1. \quad (4)$$

Besides, the operators $\hat{a},\ \hat{a}^+$ commute with operators $\hat{b},\ \hat{b}^+$. These relations are crucial for the algebraic calculation.

All operators in equation (2) can be expressed via the annihilation and creation operators as following formulae:

$$\hat{T} = \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} = \omega\left(\hat{a}\hat{b} + \hat{a}^+\hat{b}^+ - \hat{a}^+\hat{a} - \hat{b}^+\hat{b} - 1\right), \tag{5}$$

$$\hat{R} = u^2 + v^2 = \frac{1}{\omega}\left(\hat{a}\hat{b} + \hat{a}^+\hat{b}^+ + \hat{a}^+\hat{a} + \hat{b}^+\hat{b} + 1\right), \tag{6}$$

$$\hat{l}_z = -\frac{i}{2}\left(v\frac{\partial}{\partial u} - u\frac{\partial}{\partial v}\right) = \frac{1}{2}\left(\hat{a}^+\hat{a} - \hat{b}^+\hat{b}\right). \tag{7}$$

These operators are easy to work with the harmonic wave functions, which can be written in the algebraic form as eigenvectors of the neutral operators $\hat{a}^+\hat{a}$, $\hat{b}^+\hat{b}$:

$$|k,m\rangle = \frac{1}{\sqrt{(k+m)!(k-m)!}}(\hat{a}^+)^{k+m}(\hat{b}^+)^{k-m}|0\rangle. \tag{8}$$

Here, the vacuum state $|0\rangle$ is defined by the equation

$$\hat{a}|0\rangle = 0, \quad \hat{b}|0\rangle = 0. \tag{9}$$

Because our system has the conserved angular momentum, we pick up for the basis set (8) only the wave vectors, which are the eigenvectors of the operator $\hat{l}_z$. From the form of $\hat{l}_z$ via the annihilation and creation operators shown in (7), it is easy to verify that vectors (8) are eigenvectors corresponding to the eigenvalues $m = 0, \pm1, \pm2, \ldots$. Then, the rest running index has the values: $k = |m|, |m|+1, |m|+2, \ldots$

By using the commutation relations (4) and the vacuum state definitions (9), we can calculate all the matrix elements of operators in equation (2). Particularly, the elements:

$$T_{jk} = \omega^{-1}\langle j,m|\hat{T}|k,m\rangle, \qquad R_{jk} = \omega\langle j,m|\hat{R}|k,m\rangle,$$

$$(R^3)_{jk} = \omega^3\langle j,m|\hat{R}^3|k,m\rangle, \qquad (V_K)_{jk} = \langle j,m|\omega\hat{V}_K|k,m\rangle$$

are given explicitly in Ly et al. (2023), and are useful for our application in the next sections.

2.3. Rayleigh-Schrödinger perturbation theory

The perturbation theory was conventionally developed for the typical Schrödinger equation $\hat{H}\psi = E\psi$. However, our equation (2) has a different form

$$\hat{H}\psi(u,v) = E\,\hat{R}\psi(u,v), \tag{10}$$

requiring a modified theory, which we will discussed in this section. We note that equation (10) is from equation (2) with changing $E - \frac{1-\rho}{1+\rho}\frac{m\gamma}{2} \to E$, for convenience.

The first step is to split the Hamiltonian $\hat{H}$ and operator $\hat{R}$ into two terms as

$$\hat{H} = \hat{H}_0 + \beta\hat{V}, \qquad \hat{R} = \hat{R}_0 + \beta\hat{R}_V. \tag{11}$$

The main terms $\hat{H}_0$ and $\hat{R}_0$ include all neutral operators, and the rest of the non-neutral operators $\hat{V}$, $\hat{R}_V$ can be treated as perturbative. Here, as shown later, energies in the zero-

order approximation are non-degenerated. The perturbative parameter $\beta \ll 1$ is used to denote the perturbativeness of operators $\hat{V}, \hat{R}_V$. This parameter is entered formally to establish formulas of perturbation corrections; thus, we will put the value $\beta = 1$ at the last step.

The second step is to calculate the matrix elements of the related operators. First, we use functions (8), $|k,m\rangle$ $(k = |m|, |m|+1, |m|+2, ...)$, that are normalized and orthogonal for the basis set. Therefore, the matrix elements of operators $\hat{H}_0$, $\hat{R}_0$, $\hat{V}$, and $\hat{R}_V$ have the following properties when $j \neq k$:

$$\langle k,m|\hat{H}_0|j,m\rangle = 0,\ \langle k,m|\hat{R}_0|j,m\rangle = 0,\ \langle k,m|\hat{V}|j,m\rangle = v_{kj},\ \langle k,m|\hat{R}_V|j,m\rangle = r_{kj}. \quad (12)$$

In the case of $j = k$, we have

$$\langle k,m|\hat{H}_0|k,m\rangle = h_{kk},\ \langle k,m|\hat{R}_0|k,m\rangle = r_{kk},\ \langle k,m|\hat{V}|k,m\rangle = 0,\ \langle k,m|\hat{R}_V|k,m\rangle = 0. \quad (13)$$

In our case, all the elements h_{kk}, r_{kk}, v_{kj}, r_{kj} can be expressed via the calculated matrix elements T_{jk}, R_{jk}, $(R^3)_{jk}$, $(V_K)_{jk}$. We note that the separation of operators in formulas (11) is just for constructing the theory. In practice, we only need to calculate the matrix elements by the formulae (12) and (13) and then apply them to the calculation scheme for the perturbative corrections.

The third step is to calculate zeroth-order energies and wave functions, which can be yielded from the zeroth-order approximation

$$\hat{H}_0|\psi_{nm}^{(0)}\rangle = E_{nm}^{(0)}\,\hat{R}_0|\psi_{nm}^{(0)}\rangle. \quad (14)$$

Because the operators $\hat{H}_0$ and $\hat{R}_0$ contain only the neutral operators $\hat{a}^+\hat{a}$, $\hat{b}^+\hat{b}$, the zero-order approximation wave vectors are $|\psi_{nm}^{(0)}\rangle = |n,m\rangle$ corresponding to the zeroth-order energies:

$$E_{nm}^{(0)} = \varepsilon_{nm} = \frac{h_{nn}}{r_{nn}}. \quad (15)$$

Next, we get the first order of wave functions and energies in the form of

$$|\psi_{nm}^{(1)}\rangle = |n,m\rangle + \beta|\Delta\psi_{nm}^{(1)}\rangle, \qquad E_{nm}^{(1)} = \varepsilon_{nm} + \beta\,\Delta E_{nm}^{(1)}. \quad (16)$$

Substituting (16) into equation (10), using the constraints from (11), (14), and (15), and simplifying the β parameter to the first-order approximation, we get

$$\left(\hat{H}_0 - \varepsilon_{nm}\hat{R}_0\right)|\Delta\psi_{nm}^{(1)}\rangle + \left(\hat{V} - \varepsilon_{nm}\hat{R}_V\right)|n,m\rangle - \Delta E_{nm}^{(1)}\,\hat{R}_0|n,m\rangle = 0. \quad (17)$$

From (17), we can find the corrections $|\Delta\psi_{nm}^{(1)}\rangle$ and $\Delta E_{nm}^{(1)}$ of wave function and energy, respectively. Indeed, we multiply both sides (19) by the wave function $|\psi_{nm}^{(0)}\rangle = |n,m\rangle$ and integrate all over the domain (u,v). As a result, we have

$$\left\langle n,m\right|\hat{H}_0-\varepsilon_{nm}\hat{R}_0\left|\Delta\psi_{nm}^{(1)}\right\rangle+\left\langle n,m\right|\hat{V}-\varepsilon_{nm}\hat{R}_V\left|n,m\right\rangle=\Delta E_{nm}^{(1)}\left\langle n,m\right|\hat{R}_0\left|n,m\right\rangle. \quad (18)$$

Due to operators $\hat{H}_0$ and $\hat{R}_0$ being Hermitian, the first term can be calculated by using (14), and as a result, it equals zero. Moreover, with the properties of operators $\hat{V}$ and $\hat{R}_V$ shown in the equations (12) and (13), we can conclude that other terms of (18) are also equal to zero, and thus the first-order correction of energy has vanished, i.e.

$$\Delta E_{nm}^{(1)}=0. \quad (19)$$

At this point, we are able to calculate the first-order correction of the wave function from equation (17) by plugging equation (19) in it. We achieve

$$\left|\Delta\psi_{nm}^{(1)}\right\rangle=-\frac{1}{\hat{H}_0-\varepsilon_{nm}\hat{R}_0}\left(\hat{V}-\varepsilon_{nm}\hat{R}_V\right)\left|n,m\right\rangle. \quad (20)$$

The basic set is orthogonal; thus, we can express functions $\hat{V}\left|n,m\right\rangle$ and $\hat{R}_V\left|n,m\right\rangle$ by the basic set and calculate the expansion coefficients in terms of matrix elements to get

$$\hat{V}\left|n,m\right\rangle=\sum_{\substack{j=|m|\\ j\neq n}}^{+\infty}v_{jn}\left|j,m\right\rangle,\quad \hat{R}_V\left|n,m\right\rangle=\sum_{\substack{j=|m|\\ j\neq n}}^{+\infty}r_{jn}\left|j,m\right\rangle. \quad (21)$$

By plugging (21) into (20), we have first-order correction of the wave function as follows

$$\left|\Delta\psi_{nm}^{(1)}\right\rangle=-\sum_{\substack{j=|m|\\ j\neq n}}^{+\infty}\frac{v_{jn}-\varepsilon_{nm}r_{jn}}{h_{jj}-\varepsilon_{nm}r_{jj}}\left|j,m\right\rangle. \quad (22)$$

It is necessary to note that the eigenvalue of equation (14) is non-degenerate, so the denominator in formula (22) is not equal to zero. Otherwise, we need to establish the formula using the degenerate Rayleigh-Schrödinger perturbation theory. Finally, we move to the second-order approximation of energy and wave function by the expansion of

$$\left|\psi_{nm}^{(2)}\right\rangle=\left|n,m\right\rangle+\beta\left|\Delta\psi_{nm}^{(1)}\right\rangle+\beta^2\left|\Delta\psi_{nm}^{(2)}\right\rangle,\qquad E_{nm}^{(2)}=\varepsilon_{nm}+\beta^2\,\Delta E_{nm}^{(2)}. \quad (23)$$

Plugging (23) into equation (10) with the operators in the form of (11) and expanding the equation using (23) up to β^2, we yield

$$\left(\hat{H}_0-\varepsilon_{nm}\hat{R}_0\right)\left|\Delta\psi_{nm}^{(2)}\right\rangle+\left(\hat{V}-\varepsilon_{nm}\hat{R}_V\right)\left|\Delta\psi_{nm}^{(1)}\right\rangle-\Delta E_{nm}^{(2)}\,\hat{R}_0\left|n,m\right\rangle=0. \quad (24)$$

Following the same steps as for the first-order approximation, we get the formulas of the second-order correction of energy and wave function as follows:

$$\Delta E_{nm}^{(2)}=-\sum_{\substack{j=|m|\\ j\neq n}}^{+\infty}\frac{\left(v_{jn}r_{nn}-h_{nn}r_{jn}\right)^2}{\left(h_{jj}r_{nn}-h_{nn}r_{jj}\right)^2 r_{nn}^{\ 2}}, \quad (25)$$

$$\left|\Delta\psi_{nm}^{(2)}\right\rangle=-\sum_{\substack{j=|m|\\ j\neq n}}^{+\infty}\sum_{\substack{k=|m|\\ k\neq n}}^{+\infty}\frac{\left(v_{jn}r_{nn}-h_{nn}r_{jn}\right)\left(v_{kj}r_{nn}-h_{nn}r_{kj}\right)}{\left(h_{jj}r_{nn}-h_{nn}r_{jj}\right)\left(h_{kk}r_{nn}-h_{nn}r_{kk}\right)}\left|k,m\right\rangle. \quad (26)$$

2.4. Variational parameter

We have introduced a parameter ω while defining the annihilation and creation operators $\hat{a}$, $\hat{a}^+$, $\hat{b}$, $\hat{b}^+$ in subsection 2.2. In principle, this *variational parameter does not affect the final results of magnetoexciton energies or wavefunctions but manipulates the convergence speed of numerical calculations. The variational parameter can be chosen appropriately to adjust the magnitude relationship between the perturbation and non-perturbation terms of matrix elements, thus modifying the convergence rate of calculations at high orders.*

One way to identify the parameter ω is by taking the derivative of the zeroth-order energy with respect to ω because of its independence from the *variational parameter*

$$\frac{\partial E_{nm}^{(0)}}{\partial \omega} = 0, \tag{27}$$

where

$$E_{nm}^{(0)} = \frac{\omega^2}{2} + \frac{1-\rho}{1+\rho}\frac{m\gamma}{2} + (5n^2+5n+3-3m^2)\frac{\gamma^2}{4\omega^2} + \frac{(V_K)_{nm}}{2n+1}. \tag{28}$$

The equation (27) can be solved numerically. Furthermore, constraint (27) can be interpreted as a global minimum of $E_{nm}^{(0)}$ for each state and value of the magnetic field. Therefore, we can find the appropriate parameter ω corresponding to the state and the magnetic field strength. The discussion on choosing ω is also discussed by Ly et al. (2022).

3. *Results and Discusion*

3.1. Exciton energies

Magnetoexciton energies at second-order correction are defined by

$$E_{nm}^{(2)}(B) = E_{nm}^{(0)} + \Delta E_{nm}^{(2)} \tag{29}$$

in which $E_{nm}^{(0)}$ and $\Delta E_{nm}^{(2)}$ are calculated by formulas (15) and (25), respectively. The variational parameter is given by solving equation (27). To obtain magnetoexciton energies, we use the programming language Python for calculating. It is worth noting that the infinite sum in equation (25) is limited to the first 100 terms, which is sufficient to achieve accurate magnetoexciton energies up to 8 decimal digits. Here, we use input parameters for monolayer WSe_2 encapsulated by boron nitride (h-BN): mass ratio $\rho = 0.94$, exciton reduced mass $\mu = 0.2039\,\mathrm{m_e}$, screening length $r_0 = 4.2086\,\mathrm{nm}$, and dielectric constant of the surrounding material $\kappa = 4.5$. The magnetic field is applied up to 10 Tesla. Some exciton energies for different states are presented in Table 1, followed by the relative errors compared with the data reported by Ly et al. (2023).

It becomes apparent that the relative errors of each state tend to rise gradually as the magnetic field strength increases (Table 1). Magnetoexciton energies in the uniform magnetic field up to 10 Tesla in 1s, $2p^+$, and $2p^-$ states have significantly low relative errors, lower than 0.3%. Particularly, at a magnetic field strength of 10 Tesla, the relative error of

the $2p^-$ state attains its minimum value at 0.0002 %, demonstrating a high level of agreement with the energy values reported in Ly et al. (2023), up to six decimal places. For 2s and 3s, the relative errors maintain lower than 5% in the low magnetic field.

Table 1. *Magnetoexciton energies (eV) for different states. The results are compared with data from Ly et al. (2023)*

	1s			**2s**		
B (Tesla)	$E^{(2)}(B)$	$E(B,T=0)$ (Ly et al., 2023)	$\delta_{B,T=0}$	$E^{(2)}(B)$	$E(B,T=0)$ (Ly et al., 2023)	$\delta_{B,T=0}$
0	-0.16796063	-0.16855204	0.4 %	-0.03700082	-0.03855389	4.0 %
0.1	-0.16796062	-0.16855204	0.4 %	-0.03700075	-0.03855384	4.0 %
1	-0.16796028	-0.16855176	0.4 %	-0.03699422	-0.03854895	4.0 %
10	-0.16792612	-0.16852370	0.4 %	-0.03635477	-0.03806622	4.5 %

	$2p^-$			**2p+**		
B (Tesla)	$E^{(2)}(B)$	$E(B,T=0)$ (Ly et al., 2023)	$\delta_{B,T=0}$	$E^{(2)}(B)$	$E(B,T=0)$ (Ly et al., 2023)	$\delta_{B,T=0}$
0	-0.04977768	-0.04978157	0.008 %	-0.04977768	-0.04978157	0.008 %
0.1	-0.04977854	-0.04978236	0.008 %	-0.04977678	-0.04978073	0.008 %
1	-0.04978406	-0.04978737	0.007 %	-0.04976650	-0.04977101	0.009 %
10	-0.04962667	-0.04962675	0.0002 %	-0.04945159	-0.04946320	0.02 %

	3s		
B (Tesla)	$E^{(2)}(B)$	$E(B,T=0)$ (Ly et al., 2023)	$\delta_{B,T=0}$
0	-0.01619889	-0.01655162	2.1 %
0.1	-0.01619864	-0.01655136	2.1 %
1	-0.01616776	-0.01652562	2.2 %
10	-0.01343757	-0.01420413	5.4 %

3.2. Diamagnetic coefficient

The diamagnetic coefficient is a quantity related to the diamagnetic shift of magnetoexciton energy. The coefficient is proportional to the quadratic of magnetic field strength and is generally expressed through the equation

$$\sigma_{nm} = \frac{1}{2}\lim_{B\to 0}\frac{\partial^2 E_{nm}}{\partial B^2}. \tag{30}$$

First, we must consider magnetoexciton energy in a weak magnetic field to obtain the diamagnetic coefficient, where the typical length is much greater than the mean magnetoexciton radius. Fortunately, the modulated perturbation method allows us to

calculate energy numerically in the whole range of magnetic fields without any changes in the energy equations, which is quite convenient than the traditional perturbation theory.

The zeroth-order energy equation given by the modulated perturbation theory (28) can be written in a dimensional form as

$$E_{nm}^{(0)} = a_0 + b_0 B^2 + c_0 B, \tag{31}$$

where a_0, arising from neutral operators in Hamiltonian, is independent of the magnetic field. At the same time, other coefficients, b_0 and c_0, are proportional to quadratic and linear magnetic field strength, respectively. Here, the magnetic field unit is Tesla, and the energy unit is eV. The coefficient c_0 only exists when considering non-s-states due to its dependence on the magnetic quantum number m. According to the definition of the diamagnetic coefficient, the coefficient b_0 is indeed the zeroth-order diamagnetic coefficient of magnetoexciton when taking the second-order derivative of the equation (31) with respect to the magnetic field.

Similarly, we must rewrite the second-order energy equation as

$$E_{nm}^{(2)} = a_2 + b_2 B^2 + c_2 B \tag{32}$$

to obtain the second-order diamagnetic coefficient. Although the equation in its original form (25) can not be directly expressed as (32), we can interpret numerical results in this form due to the similarity to the zeroth-order equation. It means that the coefficient b_2 is the second-order diamagnetic coefficient. From (31) and (32), we can use linear or quadratic regression by the least mean square method to retrieve all coefficients in both equations. By utilizing the adjusted R^2, as discussed in Kutner et al. (2005), we obtain great precision from 0.98 up to 0.99 for all states. Diamagnetic coefficients presented in Table 2 are well comparable with theoretical calculations (Liu et al., 2019; Ly et al., 2023), and the experimental results from Stier et al. (2018).

Table 2. *Diamagnetic coefficients in different states are given in unit of* $\mu eV/Tesla^2$ *by the modulated perturbation method compared with experimental and other theoretical data*

	1s	**2s**	**2p$^-$**	**2p$^+$**	**3s**
σ_{nm} (Stier et al., 2018)	0.31 ± 0.02	4.6 ± 0.2	-	-	22 ± 2
σ_{nm} (Liu et al., 2019)	0.31	4.86	-	-	24.2
σ_{nm} (Ly et al., 2023)	0.289	5.039	2.429	2.429	26.53
$\sigma_{nm}^{(0)}$	0.358	3.229	2.564	2.564	17.241
$\sigma_{nm}^{(2)}$	0.317	4.855	2.419	2.414	23.871

4. Conclusion

The modulated perturbation method is developed successfully to calculate numerically magnetoexciton energies at the ground and some low-lying states in the entire range of

magnetic field up to 10 Tesla. The numerical energies achieve a precision level of up to 8 decimal places and are comparable to the exact numerical results. We also use the linear and quadratic regression by the least mean square method to obtain the diamagnetic coefficient of magnetoexciton in several states. The results are similar with other recent studies and even show some advantages compared to other methods.

The high accuracy of the second-order approximation of the modulated perturbation theory obtained in the present paper suggests that this method should be applied to achieve analytical exciton energies. This proposal is ongoing, and we will publish the results elsewhere.

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NĂNG LƯỢNG VÀ HỆ SỐ NGHỊCH TỪ CHO EXCITON TRONG ĐƠN LỚP WSe_2

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TÓM TẮT

Exciton hai chiều trong đơn lớp TMDC (transition-metal dichalcogenides) đặt trong từ trường đều là một bài toán hấp dẫn đối với nghiên cứu thực nghiệm lẫn lí thuyết trong thập kỉ vừa qua do có tính ứng dụng cao trong các thiết bị quang-điện tử. Đặc biệt hệ số nghịch từ của exciton trong đơn lớp TMDC nhận được nhiều sự quan tâm, cụ thể là đơn lớp WSe_2 được kẹp bởi boron nitride (h-BN). Tuy nhiên, sự chênh lệch giữa các tính toán lí thuyết và đo đạc thực nghiệm đối với các đại lượng của vật liệu đòi hỏi cần phải có nhiều sự cải tiến về mặt lí thuyết. Trong công trình này, chúng tôi sử dụng phương pháp nhiễu loạn có điều tiết bằng cách kết hợp lí thuyết nhiễu loạn Rayleigh-Schrödinger cùng với phép biến đổi Levi-Civita và thêm vào một tham số tự do. Phương pháp này có lợi thế trong việc xác định hệ số nghịch từ exciton ở gần đúng bậc hai. Các kết quả hệ số nghịch từ thu được cho thấy sự phù hợp tốt với các công trình hiện nay.

Từ khóa: hệ số nghịch từ; exciton; phương pháp nhiễu loạn có điều tiết; TMDC