Thermo-induced effect on magnetoexciton energy spectra in monolayer transition-metal dichalcogenides

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It is widely comprehended that the temperature may cause phonon-exciton scattering, enhancing the energy level’s linewidth and leading to some spectrum shifts. However, in the present Letter, we suggest a different mechanism that allows the thermal motion of the exciton’s center of mass (c.m.) to affect the magnetoexciton energies in monolayer dichalcogenides (TMDCs). By the non-trivial but precise separation of the c.m. motion from an exciton in monolayer TMDC with a magnetic field, we obtain an equation for the relative motion containing a motional Stark term proportional to the c.m. pseudomomentum, related to the temperature of the exciton gas but neglected in the previous studies. Solving the Schrödinger equation without omitting the motional Stark potential at room temperature shows a few meV thermal-magnetic shifts in the exciton energies, significant enough for experimental detection. Moreover, the thermo-induced effect causes an increase in excitation radius and diamagnetic coefficient and enhances the exciton lifetime as a consequence. Surprisingly, the thermo-induced potential breaks the system’s SO(2) symmetry, conducting new peaks in the exciton absorption spectra at room temperature besides those of the s-states. This mechanism could be extended for other magneto-quasiparticles such as trions and biexcitons.

Keywords: exciton, transition-metal dichalcogenides, finite temperature, motional Stark effect potential, thermo-induced effect

Introduction — During the last two decades, monolayer transition-metal dichalcogenides (TMDCs) have become hot spots for studying the formation of excitons because of their unique property of electron-hole interaction [1–4]. Unlike three-dimensional exciton in novel semiconductors, neutral exciton in these monolayer TMDCs is thermally stable at room temperature, even for the Rydberg states. Their high binding energy provides beneficial optical properties in both UV and IR ranges [5–9]. Especially, exciton energy spectra under the presence of a constant magnetic field have been of great interest recently both in experimental observations and theoretical studies due to their incredible potential in retrieving several physical quantities of monolayer TMDCs, such as effective masses of electron and hole, the g-Landé factors, and 2D polarizability [10–16, 18–21]. Therefore, it is essential to qualitatively (and quantitatively, if possible) comprehend the influences of external factors like temperature on the energy spectra of magnetoexciton in the monolayer TMDCs.

Schrödinger equation — To consider the thermal effect, we need to solve the Schrödinger equation of the electron-hole pair in the framework of the effective mass approximation, where a Wannier exciton in a monolayer TMDC is described as a two-dimensional system of one electron and one hole interacting with each other by the potential $\hat{V}_{h-e}(r)$ in the Oxy plane, as shown in Fig. 1. Because of the two-dimensional many-particle effect, the interaction potential $\hat{V}_{h-e}$ is no longer Coulombic but screened and described by the Keldysh potential [1, 2, 22, 23]. One required task before solving the Schrödinger equation is to separate the movement of the electron-hole center of mass (c.m.) with the coordinate R. However, for a two-body system such as an exciton in a magnetic field $\mathbf{B} = B\mathbf{e}_z$, the c.m. dynamics can not be removed totally from the equation describing the electron-hole relative motion. The variable-separation procedure for this system is no longer trivial because the magnetic field breaks the system’s translation symmetry, which leads to the nonconservation of the total momentum $P$ of the electron-hole pair. Fortunately, there is an alternative constant of motion, pseudomomentum $\hat{P}_0 = \hat{P} - \frac{q}{2} \mathbf{r} \times \mathbf{B}$, commuting with the system’s Hamiltonian, i.e., $[\hat{P}_0, \hat{H}_X] = 0$. Using this conservative quantity, one can obtain an equation for the relative motion [24–26]. In this case, the wave
function can be written as
\[ \Psi_K(R, r) = e^{\frac{i}{\hbar}(K + \frac{e}{c}\mathbf{B} \times r)} r \psi_K(r), \]  
(1)
where \( K \) is an eigenvector of operator \( \hat{P}_0 \). The wave function for relative motion \( \psi_K(r) \) is obtained by solving the Schrödinger equation
\[
\left\{ \begin{array}{l}
\hat{p}^2 \left( \frac{1}{2\mu} \right) + \frac{1 - \sigma}{2} \frac{eB}{\mu} z + \frac{e^2B^2}{8\mu} r^2 + \hat{V}_{h-e}(r) \\
- \frac{e}{M} (\mathbf{B} \times \mathbf{K}) \cdot \mathbf{r} - E \end{array} \right\} \psi_K(r) = 0.
\]  
(2)
with the total mass \( M = m^*_e + m^*_h \), the exciton reduced mass \( \mu = m^*_e m^*_h / (m^*_e + m^*_h) \), and the ratio of masses \( \sigma = m^*_e / m^*_h \). Here, \( m^*_e \) and \( m^*_h \) are the effective masses of the electron and hole; \( e \) is the elementary charge with the positive value; \( \hat{p} \) and \( \hat{L}_z \) are the operators of the momentum and angular momentum of the relative motion. A detailed derivation of Eq. (S-49) is given in Suppl. [27].

For the exciton in monolayer TMDCs such as WSe\(_2\) as considered in this work, the exciton reduced mass \( \mu = 0.20 \times m_e \), mass ratio \( \sigma = 0.94 \), total mass \( M = 0.80 \times m_e \) (\( m_e \) - electron mass), and the Keldysh potential’s parameters (the average dielectric constant of the surrounding material \( \kappa = 4.5 \), screening length \( r_0 = 4.21 \)) are taken from Refs. [15, 20].

Thermo-induced motional Stark potential — In equation (S-49), we consider the specific term \( V_{mS} = -\frac{\hbar}{\mu} \mathbf{B} \times \mathbf{K} \cdot \mathbf{r} \) containing the c.m. pseudomomentum \( \mathbf{K} \) and will show its relation to the temperature of the neutral exciton gas. First, we note that the density of excitons \( n_X \) in monolayer TMDCs is low, i.e., the average distance between two excitons \( 1/\sqrt{n_X} \) is much larger than the thermal wavelength \( \lambda_{th} = \sqrt{\hbar^2 / m_e k_B T} \) so that the Maxwell-Boltzmann statistics is still valid. Indeed, the density \( n_X \), i.e., the number of neutral excitons per unit area, could be modulated around \( 10^{11} - 10^{12} \) cm\(^{-2}\) in real experiments for monolayer WSe\(_2\) [28-31], which is much smaller than its limit at room temperature \( \lambda_{th}^2 = 4.3 \times 10^{12} \) cm\(^{-2}\). Then, we estimate the root-mean-square of the c.m. pseudomomentum at temperature \( T \) by the equipartition theorem as \( \sqrt{\frac{1}{3\mu}K^2} = k_B T \), where \( k_B \) is the Boltzmann constant. Instead of calculating exciton energies at each pseudomomentum value and then averaging them as \( E(K) \), we do it another way by calculating the exciton energy \( E(K) \) at the average pseudomomentum value. This approach allows the considered potential to relate to the temperature as follows
\[ V_{mS}(r) = -\frac{2k_B T}{M} eB x. \]
(3)
Here, without losing generality, we consider the case where \( \mathbf{K} \) is along the \( Oy \) axis so that vector \( \mathbf{B} \times \mathbf{K} \) is along the \( Ox \) axis. A more microscopic grounding for the thermo-induced term (S-52) is given in Suppl. [27].

The potential (S-52) influences the exciton in the same way as the Stark effect [32, 33], so we call it thermo-induced motional Stark potential. Recent theoretical studies of magnetoexciton in monolayer TMDCs always neglect this potential [14, 18, 21] that is reasonable only at zero temperature. However, the experimental observations were conducted not only at low temperatures [11, 13, 15, 16, 19, 20] but also at room temperature [9, 10, 34, 35]. Hence, the motional Stark effect arising from the thermal fluctuation of the c.m. pseudomomentum needs to be considered when calculating the energy spectra of magnetoexciton in monolayer TMDCs.

We can see that the diamagnetic term \( V_{diamag} = \frac{e^2 B^2 r^2}{8\mu} \) in the effective potential of Eq. (S-49) is quadratically proportional to the electron-hole distance and consequently dominant at the large separation of the electron-hole pair compared to the thermo-induced Stark term, which is linearly proportional to the variable \( x \). As a result, there is no tunneling effect, even considering the thermo-induced motional Stark potential. The exciton is always in its bound states, unlike the well-known LoSurd-Stark effect in the two-dimensional electron gas [36, 37] and field-induced dissociation of excitons in a TMDC [38]. Instead of tunneling, we expect the thermo-induced motional Stark potential could cause the Stark shift in the energy spectra.

Thermo-induced effect on diamagnetic coefficient and Landau levels — To see how the thermo-induced motional Stark potential affects the asymptotic behaviors of exciton energies in the limits of low and high magnetic intensities, we calculate the energies analytically by applying the perturbation theory to the Schrödinger equation (S-49). For low magnetic intensity, restricted by the condition that the typical length in the magnetic field is much larger than the average exciton radius: \( l_B = \sqrt{\hbar / eB} \gg \langle r \rangle_{nm} \), we have the energy of the \((n, m)\) quantum state in the second perturbation order as
\[ E^{(2)}_{nm}(B, T) = E^{(0)}_{nm} + \frac{1 - \sigma}{1 + \sigma} \frac{m h}{2\mu} eB + \frac{\langle r^2 \rangle_{nm}}{8\mu} e^2 B^2 - \alpha_{nm} k_B T m e^2 B^2, \]
(4)
where \( E^{(0)}_{nm} \), \( \langle r^2 \rangle_{nm} \), and \( \alpha_{nm} \) are the zero-field energy, squared radius, and polarizability of the exciton. To calculate these quantities, we need to solve the Schrödinger equation in the zeroth order of approximation. However, the solutions cannot be obtained analytically, so, we do it another way by numerically solving equation (S-49) and then fitting the obtained results to formula (S-59). The concrete values are presented in Table I for 1s, 2s, 3s, 2p\(_{-1}\), and 2p\(_{+1}\) states.

The last term in the exciton energy (S-59), the motional Stark correction, is quadratically proportional to the magnetic field. That means the thermo-induced effect contributes to the diamagnetic coefficient \( \sigma_{nm} \) de-
TABLE I. Zero-field energies, squared radius, and polarizability.

| Energy | 1s | 2s | 3s | 2p-1 | 2p+1 |
|--------|----|----|----|------|------|
| $E_{nm}^{(1)}$ (eV) | -0.1686 | -0.0386 | -0.0166 | -0.0498 | -0.0498 |
| $\langle r^2/n_m \rangle$ (nm$^2$) | 2.63 | 45.8 | 241 | 21.1 | 21.1 |
| $\alpha_{nm}$ (nm$^2$/eV) | 3.91 | -112 | -6060 | 259 | 240 |

induced corrections $\Delta \sigma$ are about 8% for 1s, 2s, 3s, 2p-1, and 2p+1 states at room temperature. The thermo-induced corrections are about 8% for 1s, 13% for 2s, and extremely high for higher states: 2p+1, 2p-1, and 3s (56%, 60%, and 130%). These are significant enough to impact experimental measurement that we should pay attention to when measuring exciton energies at finite temperatures.

Table II shows some values for the zero-temperature diamagnetic coefficient $\sigma_{nm}\tau$ and their thermo-induced corrections $\Delta \sigma_{nm}$ defined by the equation

$$\sigma_{nm}(T) = \lim_{B \to 0} \frac{1}{2} \frac{\partial^2 E_{nm}(B, T)}{\partial B^2} = \frac{e^2}{8\mu} \langle r^2 \rangle_{nm} - \frac{e^2}{M} \alpha_{nm} k_B T. \quad (5)$$

For high magnetic intensity, restricted by condition $l_B = \sqrt{\hbar/eB} \ll \langle r \rangle_{nm}$, the harmonic oscillator potential becomes dominant compared to the Rytova-Keldysk potential. In this case, the main part of the Hamiltonian is the magnetic term; therefore, we can obtain the Landau levels for energies with the thermo-induced Stark corrections by the perturbation theory as

$$E_{nm}^{(2)}(B, T) = \frac{\hbar}{2\mu} \left( 2n - |m| - 1 + \frac{1 - \sigma}{1 + \sigma} \right) eB - \frac{8\mu \beta_{nm}}{M} k_B T, \quad (6)$$

where the dimensionless coefficients $\beta_{nm}$ are independent of the temperature $T$, see details in Suppl. [27]. Because of the neglect of Coulomb interaction, the energy formula (S-64) is valid only for very high magnetic intensity, extremely higher than the laboratory limit of about 91 Tesla [20]. Nevertheless, this formula gives the right rule for thermo-induced shifts from the Landau levels $\Delta E = -\frac{8\mu \beta_{nm}}{M} k_B T$, i.e., linearly proportional to the temperature and almost independent of the magnetic field.

Thermal-magnetic shift on exciton energies — We now numerically investigate the thermo-induced effect on energy by the Feranchuk-Komarov operator method [18, 39]. The obtained energies are given in Suppl. [27] for the 1s, 2s, 3s, 2p-1, and 2p+1 states. For an illustration of the effect, Figs. 2(a) and (b) show exciton energies depending on the magnetic intensity at 0 K and 300 K.

We see that the temperature does not influence the 1s state much. At the same time, the thermo-induced effect is noticeable for the 2s and higher Rydberg states for the magnetic intensity of more than 60 Tesla. Particularly for the magnetic intensity of 90 Tesla, the energy shifts when including the temperature of 300K are shown in Table III. These shifts are big enough compared to the experimental sensitivity of 1 meV and are caused by the thermal motion of exciton in a magnetic field; thus, we call them the thermal-magnetic shifts.

**TABLE II. Zero-temperature diamagnetic coefficients and their thermo-induced corrections at room temperature in unit of $\mu eV/Tesla^2$ compared to the experimental data [15].**

| State | 1s | 2s | 3s | 2p-1 | 2p+1 |
|-------|----|----|----|------|------|
| $\sigma_{nm}$ [15] | 0.31 ± 0.02 | 4.6 ± 0.2 | 22 ± 2 | - | - |
| $\sigma_{nm}^0$ | 0.289 | 5.039 | 26.53 | 2.429 | 2.429 |
| $\Delta \sigma_{nm}$ | -0.022 | 0.637 | 34.42 | -1.469 | -1.361 |
| $|\Delta \sigma_{nm}|/\sigma_{nm}$ | 8% | 13% | 130% | 60% | 56% |

**TABLE III. Thermal-magnetic shifts in exciton energy spectrum calculated between the temperatures of 0 K and 300 K for the magnetic field of 90 Tesla.**

| State | 1s | 2s | 3s | 2p-1 | 2p+1 |
|-------|----|----|----|------|------|
| $\Delta E$ (meV) | 0.2 | 1.5 | 3.9 | 4.5 | 1.9 |

We note that the thermal-magnetic shift predicted above is comparable with the shift caused by the phonon-exciton interaction [34, 35]. For example, the polaron shift is about 15 meV at room temperature for 1s-state exciton in the monolayer TMDC as shown in Ref. [35]. Compared with this, the thermal-magnetic shift for the 1s state, which is 0.2 meV as shown in Table III, can be ignored. It means that neglecting the exciton c.m. motion in Ref. [35] is feasible in this case. However, for a higher excited state such as 3s, the thermal-magnetic
shift of 3.9 meV should be taken into account if the polaron shift are calculated within the presence of a high magnetic field. The two shifts are from different mechanisms (phonon-exciton scattering versus the thermal motion of the exciton c.m. in a high magnetic field). They can be calculated separately, and both have the right to be considered in analyzing experimental data for excited states in a high magnetic field. Also, for a high magnetic field of about 30 Tesla, as considered in Ref. [40], the fine structure energy split of excitons in monolayer TMDCs caused by the spin-magnetic interaction is up to tens of meV. Compared with this, the thermo-induced shift in the present work is relatively noticeable, and it is important to consider.

Thermo-induced symmetry-breaking and enhancement of exciton lifetime — It is well-known that the system of a two-dimensional exciton in a magnetic field, perpendicular to the monolayer TMDC plane, has the potential energy dependent on radius \( r = \sqrt{x^2 + y^2} \) only and consequently possesses the SO(2) symmetry. However, if included, the thermo-reduced motional Stark potential \( \langle 1 \rangle \), which depends on the angle \( \phi \) as \( \sim r \cos \phi \), will break this symmetry. In this case, the angular momentum \( l_z \) is not conserved, and the magnetic number \( m \) is no longer a good quantum number. The consequence is that there are no true s-states anymore, but only mixed states with \( m \neq 0 \) from the basis set functions; see Figs. 3 for the thermo-induced deformation of wave functions. More about the symmetry-breaking effect on the wave function deformation can be found in Suppl. [27].

The wave function deformation leads to the change of the exciton radius, essential for the exciton radiative lifetime \( \tau_{rad} \), which is related to the average electron-hole distance \( \langle r \rangle \) by the following scaling law \( \tau_{rad} \sim \langle r \rangle^{\xi} \) [41, 42]. The scaling factor \( \xi \) mainly depends on the dimensionality of the exciton. We roughly take the value of \( \xi \approx 3.5 \) extracted by studying exciton in hBN, diamond, and silicon provided in Ref. [42].

![FIG. 3. Deformation of wave functions due to the thermo-induced symmetry breaking.](image)

To have an analytical estimation, we get the formula for the exciton radius of s-states by the perturbation theory in the low magnetic field limit as

\[
\langle r \rangle_T = \langle r \rangle + g e^2 B^2 \frac{k_B T}{M},
\]

where the radius \( \langle r \rangle_T \) is calculated using the wave functions with thermo-induced effect. In contrast, the free-field wave functions are used to calculate \( \langle r \rangle \). The coefficient \( g \) has the following values 0.17 × 10^{-3}, 0.04, and -7.5 (nm^{3}/meV^{2}) for 1s, 2s, and 3s states, respectively. Consequently, we can get the following formula

\[
\frac{\Delta \tau_{rad}}{\tau_{rad}} = \xi \frac{\Delta \langle r \rangle}{\langle r \rangle}
\]

for the thermal correction \( \Delta \tau_{rad} \) to the exciton radiative lifetime, where \( \Delta \langle r \rangle = ge^2 B^2 \frac{k_B T}{M} \) for the low magnetic intensity. The correction \( \Delta \langle r \rangle \) should be calculated numerically for the high magnetic field. We estimate the ratio (8) for the 1s, 2s, and 3s states at room temperature and magnetic field of 90 Tesla and get the following values: 1.4%, 4.9%, and 2.1%, relatively considerable. The thermo-induced correction to the radiative lifetime (8) qualitatively agrees with the first-principle calculations and experimental observations given in Refs. [43–45] for the 1s state, meaning that it always enhances the lifetime and is linearly proportional to the temperature. The thermal motion also causes the lifetime to be enhanced for the 2s state but reduced for the 3s state. Therefore, this effect (enhancement/reduction of the lifetime) needs further investigation for higher states in our next work.

New peaks in absorption spectra due to the symmetry-breaking — Interestingly, the system’s symmetry-breaking at room temperature can lead to new peaks in the magnetoexciton absorption spectra, as shown in Fig. 4. First, we calculate the imaginary part of the susceptibility by the Elliot formula as

\[
\alpha(\omega) = C \Im \sum_{n,m} \frac{\omega |\psi_{nm}(\mathbf{r} = 0)|^2}{E_{nm} - E_g - \hbar \omega + i\hbar \tau},
\]

based on the linear response theory of exciton [46–49]. We use this quantity to estimate the absorption spectra since they are proportional. Here, the coefficient \( C \) depends on the materials’ background refractive index and interband transition dipole matrix elements. We are only interested in the general picture and thus choose \( C \) to normalize the free-field 1s state peak to 1 and then use it as a constant for all other states.

In Eq. (9), the bandgap energy is taken by \( E_g = 1890 \) meV from the experiment [15]. For calculation at room temperature, we subtract a value of 65 meV from the bandgap, contributed by the Varshni and polaron shifts, based on the recent work [35]. Besides, we also add the c.m. kinetic energy \( K^2/2M \) of 51.8 meV to the relative energy to get the total exciton energy \( E_{nm} \). Regarding the total lifetime, one usually considers both radiative
FIG. 4. Normalized optical absorption spectra at temperature of 0 K (black and dark blue) and at room temperature (red).

and non-radiative dephasing effects as $1/\tau = 1/\tau_{rad} + 1/\tau_{non.rad}$. However, we roughly estimate the exciton lifetime $\tau$ by the scaling law $\tau_{rad} \sim \langle r \rangle^4$ and fit the coefficient from the experiment data for the 1s state, which suggests the exciton lifetime around the picosecond. The thermal correction to the lifetime based on the formula (8) of about a few percent is not noticeable in Fig. 4.

Figure 4 illustrates the normalized linear optical absorption spectra for the quantum states with principal quantum numbers $n < 4$. This qualitative picture shows the appearance of new peaks when considering the thermo-induced effect. The explanation is based on the deformation of the wave functions, noting that the degeneracy lifting of the excited states and shifts of energies by the magnetic field and the thermo-induced potential also play an important role. Indeed, since the oscillation strength related to these peaks is proportional to the squared modulus of the wave functions at zero electron-hole separation, only the states associated with $|\psi_{nm}(r = 0)|^2 \neq 0$ can be determined by the linear optical absorption spectrum. For zero-temperature magnetoexciton, only the $s$-state wave functions have non-vanished oscillation strength while they vanish for all the other states such as $p$ and $d$; hence, we can only detect the exciton $s$-states from the linear optical response, see Fig. 4 (black and dark blue lines). However, because of the thermo-induced effect, the $p$ and $d$ states now become the superposition of other states, including $s$-states. Therefore, we get the signal of the $p$-and-$d$-state-exciton peaks on the linear optical absorption spectra at room temperature, as shown in Fig. 4 (red line).

In summary, by separating the center of mass motion from an exciton in monolayer transition-metal dichalcogenide WSe$_2$ with a magnetic field, we have pointed out the thermo-induced motional Stark potential on the Schrödinger equation, which was previously neglected. Based on this, we have proposed a new mechanism that the thermal motion of the exciton center of mass in a magnetic field could affect the energy spectra of the magnetoexciton. As an observation from our calculation, the thermal-magnetic shifts in the energy spectra are comparable with the polaron shifts caused by the exciton-phonon interaction, thus, should be considered for magnetoexciton energies at room temperature and can be observed by the shifts of resonance peaks on the absorption spectra. Surprisingly, the system’s symmetry-breaking at room temperature also causes the $p$-state exciton peaks to emerge on the linear optical absorption spectra, which cannot happen at zero temperature. These results provide another aspect of studying the influence of temperature on magnetoexciton and could be extended for other monolayer TMDCs such as WS$_2$. As an outlook, this mechanism could be applied to trions, biexcitons in Dirac materials, and magnetoexcitons originating from the strain-induced pseudomagnetic field.

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SEPARATION OF CENTER-OF-MASS MOTION

Hamiltonian for an electron-hole system in a magnetic field

The Hamiltonian for an electron-hole system in a magnetic field can be written as

\[ H_{ex} = \frac{1}{2m_e^*} \dot{p}_e^2 + \frac{1}{2m_h^*} \dot{p}_h^2 + \frac{eB}{2m_e^*} \dot{l}_e - \frac{eB}{2m_h^*} \dot{l}_h + \frac{e^2B^2}{8m_e^*} r_e^2 + \frac{e^2B^2}{8m_h^*} r_h^2 + \hat{V}_{h-e}(|r_h - r_e|), \]  (S-1)

where \( m_e^* \) and \( m_h^* \) are the effective masses of the electron and hole, respectively. To separate the variables, we use the center of mass (c.m.) coordinates \( \mathbf{R} = X \mathbf{i} + Y \mathbf{j} \) and the relative coordinates \( \mathbf{r} = x \mathbf{i} + y \mathbf{j} \) defined by the transformation

\[
X = \frac{m_h^*}{m_h^* + m_e^*} x_h + \frac{m_e^*}{m_h^* + m_e^*} x_e, \quad x = x_e - x_h, \\
Y = \frac{m_h^*}{m_h^* + m_e^*} y_h + \frac{m_e^*}{m_h^* + m_e^*} y_e, \quad y = y_e - y_h. 
\]  (S-2)

For the separation, we need to rewrite all the terms in Hamiltonian (S-1) in the coordinates \((\mathbf{r}, \mathbf{R})\) and, as a result, obtain the following

\[
\frac{1}{2m_e^*} \dot{p}_e^2 + \frac{1}{2m_h^*} \dot{p}_h^2 = \frac{1}{2M} \dot{\mathbf{p}}^2 + \frac{1}{2\mu} \dot{\mathbf{p}}^2, 
\]  (S-3)

\[
\frac{eB}{2m_e^*} \dot{l}_e - \frac{eB}{2m_h^*} \dot{l}_h = \frac{1 - \sigma}{1 + \sigma} eB \dot{\mathbf{l}} + \frac{e}{2M} (\mathbf{B} \times \mathbf{r}) \cdot \dot{\mathbf{p}} + \frac{e}{2\mu} (\mathbf{B} \times \mathbf{R}) \cdot \dot{\mathbf{p}}, 
\]  (S-4)

\[
\frac{1}{m_e^*} r_e^2 + \frac{1}{m_h^*} r_h^2 = \frac{1}{\mu} \mathbf{r}^2 + \frac{1}{(1 + \sigma)\mu} 2\mathbf{r} \cdot \mathbf{R} + \left( \frac{1}{\mu} \frac{3}{M} \right) \mathbf{r}^2. 
\]  (S-5)

Here, the total mass \( M \), the reduced mass \( \mu \), and the ratio of masses \( \sigma \) are defined as

\[
M = m_h^* + m_e^*, \quad \frac{1}{\mu} = \frac{1}{m_e^*} + \frac{1}{m_h^*}, \quad \sigma = m_e^*/m_h^*; 
\]  (S-6)

\( \dot{\mathbf{p}} \) is the c.m. momentum; \( \dot{\mathbf{p}} \) is the momentum of the relative motion between the electron and hole; \( \dot{\mathbf{l}} = x \dot{p}_y - y \dot{p}_x \) is the angular momentum of the relative motion on Oxy plane.

Using equations (S-3), (S-4), and (S-5), we can rewrite the Hamiltonian in the coordinate system of the center of mass as

\[
H_{ex} = \frac{1}{2\mu} \dot{\mathbf{p}}^2 + \frac{1 - \sigma}{1 + \sigma} \frac{eB}{2\mu} \dot{\mathbf{l}} + \frac{M - 3\mu}{M\mu} \frac{e^2B^2}{8} r^2 + \hat{V}_{h-e}(r) \\
+ \frac{1}{2M} \dot{\mathbf{p}}^2 + \frac{e^2B^2}{8\mu} R^2 + \frac{e^2B^2 (1 - \sigma)}{4\mu (1 + \sigma)} \mathbf{r} \cdot \mathbf{R} \\
+ \frac{e}{2\mu} (\mathbf{B} \times \mathbf{r}) \cdot \dot{\mathbf{p}} + \frac{e}{2\mu} (\mathbf{B} \times \mathbf{R}) \cdot \dot{\mathbf{p}}. 
\]  (S-7)
Pseudomomentum of the electron-hole system in a magnetic field

At first sight, Hamiltonian (S-7) is not variable-separable for the coordinates $\mathbf{R}$ and $\mathbf{r}$ because the total momentum $\hat{\mathbf{P}}$ is not conserved. However, there is another conservative quantity for the considered system [1–3], called pseudomomentum, defined as

$$\hat{\mathbf{P}}_0 = \hat{\mathbf{P}} - \frac{1}{2} e \mathbf{B} \times \mathbf{r} .$$  \hspace{1cm} (S-8)

We will insert this vector in the Hamiltonian instead of $\hat{\mathbf{P}}$. For this purpose, we first calculate the quadratic form $\hat{\mathbf{P}}^2_0$ and then express the kinetic energy operator of c.m. via $\hat{\mathbf{P}}_0$ as

$$\frac{1}{2M} \hat{\mathbf{P}}^2 = \frac{1}{2M} \hat{\mathbf{P}}^2_0 + \frac{e}{2M} (\mathbf{B} \times \mathbf{r}) \cdot \hat{\mathbf{P}}_0 + \frac{e^2 B^2}{8M} \mathbf{r}^2 .$$  \hspace{1cm} (S-9)

The other term in the Hamiltonian containing the total momentum $\hat{\mathbf{P}}$ can be expressed via $\hat{\mathbf{P}}_0$ too,

$$\frac{e}{2M} (\mathbf{B} \times \mathbf{r}) \cdot \hat{\mathbf{P}} = \frac{e}{2M} (\mathbf{B} \times \mathbf{r}) \cdot \hat{\mathbf{P}}_0 + \frac{e^2 B^2}{4M} \mathbf{r}^2 .$$  \hspace{1cm} (S-10)

Using equations (S-9) and (S-10), we rewrite the Hamiltonian (S-7) into

$$\hat{H}_{ex} = \frac{1}{2\mu} \hat{\mathbf{P}}^2 + \frac{1 - \sigma e B}{1 + \sigma 2\mu} \hat{I}^2_\sigma + \frac{e^2 B^2}{8\mu} \mathbf{r}^2 + \hat{V}_{h-e} (r)$$

$$+ \frac{1}{2M} \hat{\mathbf{P}}^2_0 + \frac{e}{M} (\mathbf{B} \times \mathbf{r}) \cdot \hat{\mathbf{P}}_0 + \frac{e^2 B^2}{8\mu} \mathbf{R}^2 + \frac{1 - \sigma e^2 B^2}{1 + \sigma 4\mu} \mathbf{R} \cdot \mathbf{r} + \frac{e}{2\mu} (\mathbf{B} \times \mathbf{R}) \cdot \hat{\mathbf{p}} ,$$  \hspace{1cm} (S-11)

which now contains $\mathbf{P}_0$ only.

We can also confirm that the pseudomomentum $\hat{\mathbf{P}}_0$ commutes with the Hamiltonian (S-11) by calculating commutators of $\hat{\mathbf{P}}_0$ with all the Hamiltonian terms. The following commutator relations

$$\left[ \hat{\mathbf{P}}_0 , \frac{e^2 B^2}{8\mu} \mathbf{r}^2 \right] = 0 , \quad \left[ \hat{\mathbf{P}}_0 , \hat{V}_{h-e} (r) \right] = 0 , \quad \left[ \hat{\mathbf{P}}_0 , \frac{e}{M} (\mathbf{B} \times \mathbf{r}) \cdot \hat{\mathbf{P}}_0 \right] = 0$$  \hspace{1cm} (S-12)

are trivially obtained because the operator $\hat{\mathbf{P}}_0$ does not contain the differential operator respecting $\mathbf{r}$. For all other terms in the Hamiltonian, we can calculate and receive the following commutators

$$\left[ \hat{\mathbf{P}}_0 , \hat{\mathbf{p}} \right] = -i \hbar e \mathbf{B} \times \hat{\mathbf{p}} , \quad \left[ \hat{\mathbf{P}}_0 , \hat{I}^2_\sigma \right] = \frac{1}{2} i \hbar e B R \frac{\mathbf{r}}{r} , \quad \left[ \hat{\mathbf{P}}_0 , \hat{R}^2 \right] = - \frac{1}{2} i \hbar \mathbf{R} ,$$

$$\left[ \hat{\mathbf{P}}_0 , \mathbf{r} \cdot \mathbf{R} \right] = -i \hbar \mathbf{r} , \quad \left[ \hat{\mathbf{P}}_0 , (e \mathbf{B} \times \mathbf{R}) \cdot \hat{\mathbf{p}} \right] = i \hbar e \mathbf{B} \times \mathbf{p} + \frac{1}{2} i \hbar e^2 B^2 \mathbf{R} .$$  \hspace{1cm} (S-13)

From equations (S-12) and (S-13), we can prove

$$\left[ \hat{\mathbf{P}}_0 , \hat{H}_{ex} \right] = 0 ,$$  \hspace{1cm} (S-14)

meaning that $\hat{\mathbf{P}}_0$ is an integral of motion, and $\hat{\mathbf{P}}_0$ and $\hat{H}_{ex}$ have mutual eigenfunctions.

Variable-separation and the Hamiltonian for the relative motion

We will use eigenfunctions of the pseudomomentum $\hat{\mathbf{P}}_0$ to separate the variables in the total Hamiltonian (S-7). For the first move, it is easy to verify that the wave function

$$\Psi (\mathbf{R} , \mathbf{r}) = \exp \left\{ \frac{i}{\hbar} \left( \mathbf{K} + \frac{e}{2} \mathbf{B} \times \mathbf{r} \right) \cdot \mathbf{R} \right\} \psi (\mathbf{r})$$  \hspace{1cm} (S-15)

is an eigenfunction of the operator $\hat{\mathbf{P}}_0$ with an eigenvector $\mathbf{K}$, i.e., satisfies the eigenvalue equation

$$\hat{\mathbf{P}}_0 \Psi (\mathbf{R} , \mathbf{r}) = \mathbf{K} \Psi (\mathbf{R} , \mathbf{r}) .$$  \hspace{1cm} (S-16)
Because of the commutation relation $\left[ \hat{P}_0, \hat{H}_{\text{ex}} \right] = 0$, we can choose $\psi(\mathbf{r})$ so that the wave function $\Psi(\mathbf{R}, \mathbf{r})$ becomes an eigenfunction of the Hamiltonian $\hat{H}_{\text{ex}}$, i.e.,

\[
\hat{H}_{\text{ex}} \Psi(\mathbf{R}, \mathbf{r}) = E_{\text{total}} \Psi(\mathbf{R}, \mathbf{r}).
\]  

(S-17)

Denoting $\hat{U} = \exp \left\{ \frac{i}{\hbar} (\mathbf{K} + \frac{e}{2} \mathbf{B} \times \mathbf{r}) \cdot \mathbf{R} \right\}$, we can rewrite equation (S-17) into

\[
\hat{H}_{\text{ex}} \hat{U} \psi(\mathbf{r}) = E_{\text{total}} \hat{U} \psi(\mathbf{r}) \rightarrow \hat{U}^{-1} \hat{H}_{\text{ex}} \hat{U} \psi(\mathbf{r}) = E_{\text{total}} \psi(\mathbf{r}).
\]  

(S-18)

The function $\psi(\mathbf{r})$, depending only on $\mathbf{r}$, can be considered as a wave function of the electron-hole relative motion. Consequently, equation (S-18) (subtracted by the pseudokinetic energy of the exciton c.m.) is the Schrödinger equation for relative motion with the Hamiltonian defined by the transformation

\[
\hat{H}_{\text{rel}} = \hat{U}^{-1} \hat{H}_{\text{ex}} \hat{U} - \frac{1}{2M} \mathbf{K}^2
\]

with the relative energy $E = E_{\text{total}} - \frac{1}{2M} \mathbf{K}^2$.

We can directly calculate all the terms of the Hamiltonian $\hat{H}_{\text{rel}}$ with the following results

\[
\hat{U}^{-1} \hat{p}^2 \hat{U} = \hat{p}^2 - (e \mathbf{B} \times \mathbf{R}) \cdot \hat{p} + \frac{1}{2} e^2 B^2 R^2,
\]

\[
\hat{U}^{-1} (e \mathbf{B} \times \mathbf{r}) \cdot \hat{p} \hat{U} = - \frac{1}{2} e^2 B^2 R^2 + (e \mathbf{B} \times \mathbf{R}) \cdot \hat{p},
\]

\[
\hat{U}^{-1} \hat{h}_z \hat{U} = \hat{h}_z - \frac{1}{2} eB \mathbf{r} \cdot \mathbf{R},
\]

\[
\hat{U}^{-1} \hat{P}_0 \hat{U} = K^2, \quad \hat{U}^{-1} (e \mathbf{B} \times \mathbf{r}) \cdot \hat{P}_0 \hat{U} = (e \mathbf{B} \times \mathbf{K}) \cdot \mathbf{r},
\]

\[
\hat{U}^{-1} \hat{r}^2 \hat{U} = \hat{r}^2, \quad \hat{U}^{-1} \hat{V}_{h,-e}(\mathbf{r}) \hat{U} = \hat{V}_{h,-e}(\mathbf{r}), \quad \hat{U}^{-1} \hat{R}^2 \hat{U} = \hat{R}^2, \quad \hat{U}^{-1} \hat{R} \hat{U} = \hat{R} \cdot \mathbf{R}.
\]  

(S-20)

From equations (S-19) and (S-20), we obtain the Hamiltonian for the relative motion between the electron and the hole as

\[
\hat{H}_{\text{rel}} = \frac{1}{2\mu} \hat{p}^2 + \frac{1 - \sigma}{1 + \sigma} \hat{h}_z + \frac{e^2 B^2}{8\mu} \hat{r}^2 + \hat{V}_{h,-e}(\mathbf{r}) - \frac{e}{M} (\mathbf{B} \times \mathbf{K}) \cdot \mathbf{r},
\]  

(S-21)

which is the Hamiltonian in equation (2) of the main text.

**THERMO-INDUCED MOTIONAL STARK POTENTIAL**

In equation (S-21), we now consider the term

\[
V_{\text{mS}} = -\frac{e}{M} (\mathbf{B} \times \mathbf{K}) \cdot \mathbf{r},
\]  

(S-22)

which was neglected in the previous works for the exciton energies in monolayer TMDCs. The term (S-22) contains the exciton c.m. pseudomomentum $\mathbf{K}$ that inspires us to establish its relation to the thermal motion of excitons in a monolayer TMDC.

Excitons in a monolayer TMDCT can be regarded as a gas of thermal motion with kinetic energy $K^2/2M$. We first compare the average distance between two excitons $\lambda_{\text{ex}} = 1/\sqrt{n_X}$ with the thermal wavelength $\lambda_{\text{th}} = \sqrt{2\pi \hbar^2/(MK_B T)}$ to justify which statistics should be applied for the kinetic energy distribution. Here, $n_X$ is the exciton density – the number of neutral excitons per unit of area; $k_B$ is the Boltzmann constant. For the Maxwell-Boltzmann statistics to be applied, the thermal wavelength should be much smaller than the average exciton distance that leads to the limit for the exciton density as

\[
\lambda_{\text{th}} \ll \lambda_{\text{ex}} \rightarrow n_X \ll n_{\text{max}} = \frac{MK_B T}{2\pi \hbar^2}.
\]  

(S-23)

For room temperature, 300K, we calculate the limit for the exciton density in monolayer WSe$_2$ where $M = 0.8 \times m_e$ and receive a result $n_{\text{max, 300K}} = 4.3 \times 10^{12} \text{cm}^{-2}$. On another side, the exciton density is modulated around $10^{11}$–$10^{12} \text{cm}^{-2}$ in real experiments for monolayer WSe$_2$ [4–7], which is much smaller than its limit $n_{\text{max, 300K}}$ at room temperature. Therefore, we can estimate the root-mean-square of the c.m. pseudomomentum at temperature $T$ by the equipartition theorem as $\sqrt{\frac{1}{2M} \mathbf{K}^2} = k_B T$.

In exciton gas, pseudomomentum $\mathbf{K}$ has an assembly of values $(K_1, K_2, ...)$ obeyed the Maxwell-Boltzmann distribution. To obtain the average energy $\overline{E}$ of different values $\mathbf{K}$, we principally need to calculate energies for each value
and then average the calculated energies. However, we can do this in another way by calculating energy at the average pseudomomentum $\overline{K} = \sqrt{K^2}$. The results must be the same $E(\overline{K}) \approx E$. The base for this assumption is the perturbation theory calculation that the thermo-induced potential leads to a small correction to the energy, which is proportional to the quantity $K^2$ as $E = E^{(0)} + b \times K^2$ so that $\overline{E} = E^{(0)} + b \times \overline{K}^2$. We also verify numerically that the two average methods (the average energy by different pseudomomentum vs. the energy at the average pseudomomentum) give the same results presented in Table S-I with diminutive differences of about 0.1 meV, except for 3s-state with about 0.5 meV difference (relative error of 0.68%).

TABLE S-I. Exciton energies (meV) in the magnetic field of 90 Tesla with different values of $K^2$ calculated for monolayer WSe$_2$ with $\tau_0 = 4.2086$ nm, $\mu = 0.2039\, m_e$, $\kappa = 4.5$. It also indicates energies averaged by $K^2$ and calculated at the average value of $K^2$. The energy differences between the two different calculation methods are in the last row.

| $K$ (h/\(a_0\)) \times 10^{-3} | $K^2$ (h$^2$/\(a_0^2\)) \times 10^{-3} | 1s | 2p$^{-1}$ | 2p$^{+1}$ | 2s | 3s |
|-----------------|-----------------|----|--------|--------|----|----|
| 0               | 0               | -165.807 | -33.280 | -31.645 | -6.750 | 68.124 |
| 5               | 0.025           | -165.808 | -33.292 | -31.657 | -6.743 | 68.148 |
| 10              | 0.100           | -165.810 | -33.329 | -31.693 | -6.721 | 68.221 |
| 15              | 0.225           | -165.813 | -33.390 | -31.752 | -6.684 | 68.339 |
| 20              | 0.400           | -165.818 | -33.479 | -31.831 | -6.634 | 68.501 |
| 25              | 0.625           | -165.824 | -33.597 | -31.927 | -6.604 | 68.700 |
| 30              | 0.900           | -165.831 | -33.748 | -32.037 | -6.564 | 69.195 |
| 35              | 1.225           | -165.839 | -33.934 | -32.157 | -6.508 | 69.478 |
| 40              | 1.600           | -165.849 | -34.158 | -32.285 | -6.432 | 69.777 |
| 45              | 2.025           | -165.860 | -34.420 | -32.417 | -6.377 | 70.086 |
| 50              | 2.500           | -165.872 | -34.722 | -32.552 | -6.304 | 70.397 |
| 55              | 3.025           | -165.886 | -35.062 | -32.690 | -6.227 | 70.706 |
| 60              | 3.600           | -165.901 | -35.343 | -32.831 | -6.154 | 71.004 |
| 65              | 4.225           | -165.917 | -35.565 | -32.976 | -6.097 | 71.304 |
| 70              | 4.900           | -165.935 | -35.849 | -33.125 | -6.040 | 71.604 |
| 75              | 5.625           | -165.954 | -36.179 | -33.280 | -5.985 | 71.904 |
| 80              | 6.400           | -165.974 | -36.559 | -33.440 | -5.928 | 72.204 |
| 85              | 7.225           | -165.995 | -36.987 | -33.608 | -5.871 | 72.504 |
| 90              | 8.100           | -166.018 | -37.431 | -33.782 | -5.814 | 72.806 |
| 95              | 9.025           | -166.042 | -37.897 | -33.965 | -5.756 | 73.104 |
| 100             | 10.000          | -166.068 | -38.394 | -34.177 | -5.699 | 73.406 |
| **Average**     | **3.417**       | **-165.896** | **-35.375** | **-32.657** | **-6.002** | **70.104** |

$E(\overline{K^2} = 3.417)$ | -165.895 | -35.284 | -32.774 | -5.956 | 70.580 |

**Difference (meV)** | 0.001 | 0.091 | 0.117 | 0.098 | 0.479 |

Consequently, from the above discussion, we can estimate the average pseudomomentum of exciton c.m. motion via temperature and rewrite the motional stark potential in the form

$$V_{ms}(r) = -\sqrt{\frac{2k_B T}{M}} eB x.$$  

(S-24)

Here, without losing generality, we consider the case where $\mathbf{K}$ is along the $Oy$ axis so that vector $\mathbf{B} \times \mathbf{K}$ is along the $Ox$ axis.

For the system of an atom in external electric and magnetic field, the consideration of the term (S-21) leads to additional contribution in the Stark effect although being originated from the magnetic field; thus called the motional Stark effect [8,9]. However, because this term is related to the thermal motion as we shown via the formula (S-24), we call it the thermo-induced motional Stark potential.
FIG. S-1. The effective potentials for relative motion in two cases: \( T = 0 \text{K} \) (black) and \( T = 300 \text{K} \) (red), i.e., without and with the motional Stark term. The difference between the potentials is noticeable for \( 2s \) and higher Rydberg states, where the exciton radius is larger than 6.5 nm.

The effective potential in Hamiltonian (S-21) consists of three terms as \( \hat{V}_{\text{eff}} = \hat{V}_{\text{diamag}} + \hat{V}_{\text{h}-\text{e}} + \hat{V}_{\text{mS}} \), where the diamagnetic term \( \hat{V}_{\text{diamag}} = \frac{e^2}{8\pi} B^2 r^2 \) is quadratic proportional to the electron-hole distance and consequently dominant at the large separation of the electro-hole pair compared to the thermo-induced motional Stark term \( \hat{V}_{\text{mS}} \), which is linearly proportional to the variable \( x \). As a result, there is no tunneling effect, even considering the thermo-induced motional Stark potential. Instead of tunneling, we expect the thermo-induced motional Stark potential causes the Stark shift in the energy spectra. This fact is also demonstrated clearly in Fig. S-1, where the inclusion of the thermal effect causes a higher raising in the effective potential.

FERANCHUK-KOMAROV OPERATOR METHOD FOR MAGNETOEXCITON ENERGIES UNDER INFLUENCE OF THERMO-INDUCED STARK POTENTIAL

Schrödinger equation in the formalism of creation and annihilation operators

Magnetoo exciton under the influence of thermo-induced Stark potential is described by the Schrödinger equation (2) in the main text. We rewrite it in a dimensionless form where the energy \( E \) and the coordinates \( x, y \) are given in the effective Hartree unit \( 2R_y^* = \mu e^4/16\pi^2\varepsilon_0^3\hbar^2 \) and the effective Bohr radius \( a_0^* = 4\pi\varepsilon_0\hbar^2/\mu e^2 \), respectively; the dimensionless magnetic intensity \( \gamma \) is related to the magnetic field by the equation \( B = 2\gamma \times \mu h R_y^*/e \). Then the Levi-Civita transformation \([27]\)

\[
x = u^2 - v^2, \quad y = 2uv
\]

is applied to the dimensionless Schrödinger equation to rewrite it in the \((u, v)\) space as

\[
\left\{ -\frac{1}{8} \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) + \left( \frac{1 - \sigma \gamma}{1 + \sigma} \right) \left( \int_z - E \right) (u^2 + v^2) + \frac{\gamma^2}{8} (u^2 + v^2)^3 \\
+ \frac{\sqrt{2} \sigma \theta}{1 + \sigma} \gamma (u^4 - v^4) + V(u, v) \right\} \psi(u, v) = 0,
\]

where \( \theta = k_B T/2R_y^* \) is dimensionless temperature; and \( V(u, v) = (u^2 + v^2) V_{RK} \). Here, from now on, we use the notation \( V_{RK} \) for the interaction potential of the electron and hole \( \hat{V}_{\text{h}-\text{e}} \). Also, for convenience in calculations, we
rewrite the potential \( V(u, v) \) in the Laplace transform \([28]\) as

\[
V(u, v) = -\frac{1}{\kappa} \int_{0}^{+\infty} \frac{dq}{\sqrt{1 + \alpha^2 q^2}} e^{-q(u^2 + v^2)} (u^2 + v^2),
\]

(S-27)

where the dimensionless parameter \( \alpha = r_0 / \kappa a_0^2 \) is used instead of the screening length \( r_0 \). In equations (S-26) and (S-27), we have used the formulas

\[
r = u^2 + v^2, \quad \hat{l}_z = -\frac{i}{2} \left( \frac{\partial}{\partial u} - u \frac{\partial}{\partial v} \right)
\]

(S-28)

obtained by the Levi-Civita transformation (S-25) for distance \( r \) and angular momentum \( \hat{l}_z \).

Equation (S-26) is similar to those describing a two-dimensional anharmonic oscillator, suggesting we use the harmonic oscillator wave functions as a basis set and calculate necessary matrix elements by the algebraic approach based on annihilation and creation operators, well-known as the Feranchuk-Komarov operator method in Refs. [11, 29]. The first step is to rewrite the equation in the presentation of annihilation and creation operators, defined as

\[
\hat{a} = \frac{1}{\sqrt{2}} (\hat{1} - i \hat{\beta}), \quad \hat{a}^+ = \frac{1}{\sqrt{2}} (\hat{1} + i \hat{\beta}), \quad \hat{b} = \frac{1}{\sqrt{2}} (\hat{1} + i \hat{\beta}), \quad \hat{b}^+ = \frac{1}{\sqrt{2}} (\hat{1} - i \hat{\beta}),
\]

(S-29)

where

\[
\hat{\alpha} = \sqrt{\frac{\omega}{2}} \left( u + \frac{\omega}{\partial u} \right), \quad \hat{\beta} = \sqrt{\frac{\omega}{2}} \left( v + \frac{\omega}{\partial v} \right),
\]

(S-30)

Here, \( \omega \) is a free parameter that manipulates the convergence rate of numerical calculations and does not affect the final energy spectrum. This parameter has been introduced and discussed in many references such as [11, 29] and references therein. These operators must obey the following commutation relations

\[
[\hat{a}, \hat{a}^+] = [\hat{b}, \hat{b}^+] = 1, \quad [\hat{a}, \hat{a}^+] = [\hat{b}, \hat{b}^+] = 0,
\]

(S-31)
typical for annihilation and creation operators.

All the operators of Eq. (S-26) can be presented in terms of creation and annihilation operators as

\[
- \left( \frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2} \right) = \omega \left( -\hat{a} \hat{b} - \hat{a}^+ \hat{b}^+ + \hat{a}^+ \hat{a} + \hat{b}^+ \hat{b} + 1 \right) \equiv \omega \hat{T},
\]

\[
\hat{l}_z = \frac{1}{2} \left( \hat{a}^+ \hat{a} - \hat{b}^+ \hat{b} \right),
\]

\[
u^2 + v^2 = \frac{1}{\omega} \left( \hat{a} \hat{b} + \hat{a}^+ \hat{b}^+ + \hat{a}^+ \hat{a} + \hat{b}^+ \hat{b} + 1 \right),
\]

\[
u^4 - v^4 = \left( \hat{a}^+ \hat{a}^+ + \hat{b}^+ \hat{b}^+ + \hat{a} \hat{b} + \hat{b}^+ \hat{a}^+ + 2 \hat{a} \hat{b} + 2 \hat{b}^+ \hat{a} + 2 \hat{a}^+ \hat{b} + 1 \right).
\]

(S-32)

Therefore, Eq. (S-26) is expressed as a secular equation

\[
\hat{H} |\psi\rangle - E \hat{R} |\psi\rangle = 0,
\]

(S-33)
in which the explicit expressions of \( \hat{H} \) and \( \hat{R} \) are given as

\[
\hat{R} = \hat{a}^+ \hat{a} + \hat{b}^+ \hat{b} + 1 + \hat{a} \hat{b} + \hat{a}^+ \hat{b}^+,
\]

(S-34)

\[
\hat{H} = \frac{\omega^2}{8} \hat{T} + \frac{1 - \sigma \gamma}{1 + \sigma^2 \gamma^2} \hat{R} \hat{l}_z + \frac{\gamma^2}{8 \omega^2} \hat{R}^3 - \omega \hat{V} + \frac{\sqrt{2} \sigma \theta \gamma}{1 + \sigma \gamma} \hat{V}_{ms}.
\]

(S-35)

In Eq. (S-34), operator \( \hat{V} \) describes the Rytova-Keldysh interaction in the creation-annihilation-operator formalism and is written as the following integral

\[
\hat{V} = -\frac{1}{\kappa} \int_{0}^{+\infty} \frac{dq}{\sqrt{1 + \alpha^2 q^2}} e^{-\alpha q} \hat{R},
\]

(S-36)
while operator
\[ \hat{V}_{mS} = \left( \hat{a}^+ \hat{a}^* + \hat{b}^+ \hat{b}^* + \hat{\alpha} \hat{a} + \hat{\beta} \hat{b} + 2 \hat{\beta} \hat{\alpha} + 2 \hat{a}^+ \hat{b} \right) \left( \hat{a}^+ \hat{a} + \hat{b}^+ \hat{b} + 1 + \hat{\beta} \hat{\alpha} + \hat{\alpha}^+ \hat{\beta} \right) \] (S-37)
is of the thermo-induced motional Stark potential.

**Matrix elements**

The basis set in this method is chosen by the wave functions of the two-dimensional harmonic oscillator as
\[ |k, m, \omega \rangle = \frac{1}{\sqrt{(k + m)! (k - m)!}} \left( \hat{a}^+ \right)^{k + m} \left( \hat{b}^+ \right)^{k - m} |0 \rangle, \]
(S-38)

with the running numbers \( k = |m|, |m| + 1, |m| + 2, \ldots \) and \( m = 0, \pm 1, \pm 2, \ldots \). We note that the frequency \( \omega \) can be regarded as a free parameter and will choose its value appropriate for regulating the convergence rate of the numerical solutions. Expanding the quantum wave function by this basis set as
\[ |\psi^{(s)}(\omega) \rangle = \sum_{k=0}^{s} \sum_{m=0}^{k} C^{(s)}_{km} |k, m, \omega \rangle \] (S-39)

with \( N = (s + 1)(s + 2)/2 \) unknown coefficients \( C^{(s)}_{km} \) needed to define and then putting these coefficients \( C^{(s)}_{km} \) as a column matrix \( C \), Eq. (S-33) turns into a usual form of a generalized secular equation of the eigenproblem of an \( N \times N \)-matrix \( \mathbb{H} \) with respect to \( \mathbb{R} \) as
\[ (\mathbb{H} - E \mathbb{R}) C = 0. \] (S-40)

The matrix eigenvalue equation can be solved using subroutine dsygvx.f of the Linear Algebra Package (LAPACK) [30]. Here, it is noticed that Schrödinger equation (2) is invariant under the transformation \( x \rightarrow -x, B \rightarrow -B \); therefore, we can use only \( m \geq 0 \) in the expansion (S-39). In the wave function (S-39), we use only \( (s + 1)(s + 2)/2 \) basis set functions so that the number \( s \) can be regarded as an approximation order of the solutions. In practice, we will increment the \( (s) \)-order until getting the desired precision.

Now, the second step of the Feranchuk Komarov operator method is to calculate elements of the matrices \( \mathbb{H} \) and \( \mathbb{R} \). By algebraic calculations using the commutation relations (S-31), we find out the following useful matrix elements
\[ N^{k', m'}_{k, m} = \langle k', m', \omega | \hat{a}^+ \hat{a} + \hat{b}^+ \hat{b} \rangle |k, m, \omega \rangle = 2k \delta_{k, k'} \delta_{m, m'}, \]
\[ M^{+}_{k', m'}_{k, m} = \langle k', m', \omega | \hat{a}^+ \hat{b}^+ \rangle |k, m, \omega \rangle = \sqrt{(k + 1)^2 - m^2} \delta_{k', k+1} \delta_{m', m}, \]
\[ M^{m'}_{k', m'}_{k, m} = \langle k', m', \omega | \hat{\alpha} \hat{b} \rangle |k, m, \omega \rangle = \sqrt{k^2 - m^2} \delta_{k', k-1} \delta_{m', m}, \] (S-41)

which help us to determine matrix elements as
\[ \mathbb{R}^{k', m'}_{k, m} = \langle k', m', \omega | \hat{R} |k, m, \omega \rangle = N^{k', m'}_{k, m} + M^{+}_{k', m'}_{k, m} + M^{m'}_{k', m'}_{k, m} ; \]
\[ \mathbb{H}^{k', m'}_{k, m} = \langle k', m', \omega | \hat{H} |k, m, \omega \rangle = T^{k', m'}_{k, m} + \frac{1 - \sigma}{1 + \sigma} \frac{\gamma m}{2} (\mathbb{R})^{k', m'}_{k, m} + \frac{\gamma^2}{8 \omega^2} (\mathbb{R}^3)^{k', m'}_{k, m}, \] (S-42)

\[ -\omega (\mathbb{V}_{RK})^{k', m'}_{k, m} + \frac{\sqrt{2 \sigma \theta}}{1 + \sigma} \frac{\gamma}{2 \omega} (\mathbb{V}_{ms})^{k', m'}_{k, m}, \]

where
\[ T^{k', m'}_{k, m} = \langle k', m', \omega | \hat{T} |k, m, \omega \rangle = N^{k', m'}_{k, m} - M^{m'}_{k', m'}_{k, m} - M^{+}_{k', m'}_{k, m} \] (S-43)
and

\[
\left( R^3 \right)_{k,m}^{k',m'} = \langle k', m', \omega | \tilde{R}^3 | k, m, \omega \rangle = 2 \left( 5k^2 + 5k + 3 - 3m^2 \right) \left( 2k + 1 \right) \delta_{k',k} \delta_{m',m} + 6 \left( 5k^2 + 5k + 3 - 3m^2 \right) \sqrt{k^2 - m^2} \delta_{k',k-1} \delta_{m',m} + 3 \left( 2k - 1 \right) \sqrt{k^2 - m^2} \sqrt{(k-1)^2 - m^2} \delta_{k',k-2} \delta_{m',m} + \sqrt{k^2 - m^2} \sqrt{(k-1)^2 - m^2} \sqrt{(k-2)^2 - m^2} \delta_{k',k-3} \delta_{m',m} + 6 \left( 5k^2 + 5k + 3 - 3m^2 \right) \sqrt{(k-1)^2 - m^2} \sqrt{(k-2)^2 - m^2} \delta_{k',k-1} \delta_{m',m} + 3 \left( 2k + 3 \right) \sqrt{(k+1)^2 - m^2} \sqrt{(k+2)^2 - m^2} \delta_{k',k+1} \delta_{m',m} + \sqrt{(k+1)^2 - m^2} \sqrt{(k+2)^2 - m^2} \sqrt{(k+3)^2 - m^2} \delta_{k',k+3} \delta_{m',m}.
\]

(S-45)

The matrix elements of the Rytova-Keldysh potential are calculated as

\[
(V_{RR})_{k,m}^{k',m'} = \langle k', m', \omega | \tilde{V} | k, m, \omega \rangle = \left( 2k + 1 \right) U_{k'k} + \sqrt{k^2 - m^2} U_{k'k-1} + \sqrt{(k+1)^2 - m^2} U_{k',k+1} \right) \delta_{m',m},
\]

(S-46)

where

\[
U_{j,j'} = -\frac{1}{\kappa \alpha} \sum_{s=|m|}^{\min(j,j')} \sum_{t=0}^{j'+j-2s} (-1)^{j'+j+t} \binom{j'+j-2s}{t} \times \sqrt{\binom{j'+m}{s+m}} \sqrt{\binom{j'-m}{s-m}} \sqrt{\binom{j+m}{s+m}} \sqrt{\binom{j-m}{s-m}} \times \int_{0}^{\infty} dq \left( 1 + q \right)^{2s+t+1} \sqrt{q^2 + 1/\omega^2 \alpha^2}.
\]

(S-47)

The matrix elements associated with the thermo-induced motional Stark effect are calculated as

\[
(V_{mS})_{k,m}^{k',m'} = \langle k', m', \omega | \tilde{V}_{mS} | k, m, \omega \rangle = \sqrt{(k+m)(k+m-1)(k+m-2)(k-m) \delta_{k'+m',k+m-3} \delta_{k'-m',k-m-1}} + \sqrt{(k-m+3)(k-m+2)(k-m+1)(k+m+1) \delta_{k'+m',k+m+1} \delta_{k'-m',k-m+3}} + \sqrt{(k+m+3)(k+m+2)(k+m+1)(k-m+1) \delta_{k'+m',k+m+3} \delta_{k'-m',k-m+1}} + \sqrt{(k-m)(k-m-1)(k-m-2)(k+m) \delta_{k'+m',k+m-1} \delta_{k'-m',k-m-2}} + \sqrt{(k+m+1)(k+m+2)(4k-2m+3) \delta_{k'+m',k+m+2} \delta_{k'-m',k-m}} + 3 \sqrt{(k-m)(k+m+1)(2k+1) \delta_{k'+m',k+m+1} \delta_{k'-m',k-m-1}} + \sqrt{(k-m)(k+m-1)(2k-2m+1) \delta_{k'+m',k+m-2} \delta_{k'-m',k-m}} + \sqrt{(k-m+1)(k-m+2)(4k+2m+1) \delta_{k'+m',k+m} \delta_{k'-m',k-m}} + 3 \sqrt{(k+m)(k-m+1) \delta_{k'+m',k+m-1} \delta_{k'-m',k-m-1}}.
\]

(S-48)

**Exciton energy spectrum for magnetoe exciton in WSe₂ monolayer at zero and room temperatures**

The third step is to solve Eq. (S-33) with all the matrix elements calculated. The free parameter \( \omega \) is chosen to make the convergence rate suitable for our computing resources and the required precision of 8 decimal places. This matrix
eigenvalue equation can be solved by subroutine dsygvx.f of the Linear Algebra Package (LAPACK). We present here energies of magnetoexciton in monolayer WSe$_2$ for 1$s$, 2$s$, 2$p_{-1}$, 2$p_{+1}$, and 3$s$ states with magnetic intensity up to 500 Tesla. In the paper, we show fewer results for magnetic intensities, up to 90 Tesla produced in laboratories. We note that the method is applicable for the case with no magnetic field by dropping the thermo-induced term.

### TABLE S-II. Energies of 1$s$ states (meV) with different magnetic intensity $B$ (Tesla) at temperature 0 K and 300 K for $r_0 = 4.2086$ nm, $\mu = 0.2039$ $m_e$, $\kappa = 4.5$.

| $B$ (T) | 0 K     | 300 K   | $B$ (T) | 0 K     | 300 K   |
|---------|---------|---------|---------|---------|---------|
| 0       | -168.552041 | -168.552041 | 8       | -168.533899 | -168.535348 |
| 0.1     | -168.552037 | -168.552039 | 9       | -168.529081 | -168.530915 |
| 0.2     | -168.552030 | -168.552032 | 10      | -168.523698 | -168.525961 |
| 0.3     | -168.552015 | -168.552019 | 20      | -168.438787 | -168.447803 |
| 0.4     | -168.551995 | -168.552000 | 30      | -168.297672 | -168.317802 |
| 0.5     | -168.551969 | -168.551977 | 40      | -168.100937 | -168.136347 |
| 0.6     | -168.551938 | -168.551948 | 50      | -167.543935 | -167.621388 |
| 0.7     | -168.551901 | -168.551913 | 60      | -166.312539 | -166.662897 |
| 0.8     | -168.550907 | -168.550979 | 70      | -164.648977 | -164.920434 |
| 0.9     | -168.547504 | -168.547868 | 80      | -162.958817 | -163.312647 |
| 1       | -168.541835 | -168.542651 | 90      | -161.312539 | -161.662897 |
| 2       | -168.534134 | -168.534669 | 100     | -159.678579 | -160.032647 |
| 3       | -168.509466 | -168.509609 | 110     | -157.933924 | -158.289579 |
| 4       | -168.474989 | -168.475245 | 120     | -156.188284 | -156.548245 |
| 5       | -168.430758 | -168.431463 | 130     | -154.443639 | -154.803595 |
| 6       | -168.376843 | -168.377303 | 140     | -152.699095 | -153.059051 |

### TABLE S-III. Energies of 2$s$ states (meV) with different magnetic intensity $B$ (Tesla) at temperature 0 K and 300 K for $r_0 = 4.2086$ nm, $\mu = 0.2039$ $m_e$, $\kappa = 4.5$.

| $B$ (T) | 0 K     | 300 K   | $B$ (T) | 0 K     | 300 K   |
|---------|---------|---------|---------|---------|---------|
| 0       | -38.553893 | -38.553893 | 8       | -38.240316 | -38.199502 |
| 0.1     | -38.553843 | -38.553897 | 9       | -38.157907 | -38.106499 |
| 0.2     | -38.553935 | -38.554822 | 10      | -38.066222 | -38.015013 |
| 0.3     | -38.554348 | -38.554390 | 20      | -36.699754 | -36.438785 |
| 0.4     | -38.553102 | -38.553209 | 30      | -34.548663 | -34.038135 |
| 0.5     | -38.552657 | -38.552895 | 40      | -31.719080 | -31.101684 |
| 0.6     | -38.552114 | -38.553102 | 50      | -28.420134 | -27.487797 |
| 0.7     | -38.551471 | -38.551535 | 60      | -24.700889 | -23.574784 |
| 0.8     | -38.550730 | -38.550734 | 70      | -20.626315 | -19.345456 |
| 0.9     | -38.549890 | -38.549864 | 80      | -16.249938 | -14.848486 |
| 1       | -38.548951 | -38.548302 | 90      | -11.613374 | -10.124672 |
| 2       | -38.534134 | -38.531539 | 100     | -6.750083 | -5.202292 |
| 3       | -38.509466 | -38.503636 | 110     | -1.687376 | -0.104429 |
| 4       | -38.474989 | -38.464645 | 120     | 3.552157 | 5.150194 |
| 5       | -38.430758 | -38.414637 | 130     | 8.949610 | 10.546065 |
| 6       | -38.376843 | -38.353703 | 140     | 14.488990 | 16.070108 |
TABLE S-IV. Energies of $2p_{-1}$ states (meV) with different magnetic intensity $B$ (Tesla) at temperature 0 K and 300 K for $r_0 = 4.2086$ nm, $\mu = 0.2039$ $m_e$, $\kappa = 4.5$.

| $B$ (T) | 0 K       | 300 K      | $B$ (T) | 0 K       | 300 K      |
|---------|-----------|------------|---------|-----------|------------|
| 0       | -49.781570 | -49.781570 | 8       | -49.695186 | -49.807901 |
| 0.1     | -49.782364 | -49.782378 | 9       | -49.663271 | -49.807384 |
| 0.2     | -49.783110 | -49.783167 | 10      | -49.626753 | -49.805961 |
| 0.3     | -49.783809 | -49.783937 | 20      | -49.017308 | -49.790812 |
| 0.4     | -49.784460 | -49.784689 | 30      | -47.908661 | -49.364442 |
| 0.5     | -49.785063 | -49.785423 | 40      | -46.24801 | -48.677598 |
| 0.6     | -49.785619 | -49.786139 | 50      | -44.94648 | -47.67160 |
| 0.7     | -49.786127 | -49.786838 | 60      | -43.007928 | -46.258776 |
| 0.8     | -49.786587 | -49.787521 | 70      | -38.48709 | -42.65354 |
| 0.9     | -49.787000 | -49.788186 | 80      | -33.280459 | -38.047472 |
| 1       | -49.787365 | -49.789411 | 90      | -29.978908 | -32.788581 |
| 2       | -49.788396 | -49.794511 | 100     | -26.638298 | -29.911273 |
| 3       | -49.789802 | -49.798912 | 110     | -23.180082 | -26.933141 |
| 4       | -49.776198 | -49.802825 | 120     | -19.976804 | -24.788512 |
| 5       | -49.762993 | -49.804804 | 130     | -16.860109 | -22.64152 |
| 6       | -49.745074 | -49.806567 | 140     | -13.743314 | -20.49086 |

TABLE S-V. Energies of $2p_{+1}$ states (meV) with different magnetic intensity $B$ (Tesla) at temperature 0 K and 300 K for $r_0 = 4.2086$ nm, $\mu = 0.2039$ $m_e$, $\kappa = 4.5$.

| $B$ (T) | 0 K       | 300 K      | $B$ (T) | 0 K       | 300 K      |
|---------|-----------|------------|---------|-----------|------------|
| 0       | -49.781570 | -49.781570 | 8       | -49.695186 | -49.807901 |
| 0.1     | -49.782364 | -49.782378 | 9       | -49.663271 | -49.807384 |
| 0.2     | -49.783110 | -49.783167 | 10      | -49.626753 | -49.805961 |
| 0.3     | -49.783809 | -49.783937 | 20      | -49.017308 | -49.790812 |
| 0.4     | -49.784460 | -49.784689 | 30      | -47.908661 | -49.364442 |
| 0.5     | -49.785063 | -49.785423 | 40      | -46.24801 | -48.677598 |
| 0.6     | -49.785619 | -49.786139 | 50      | -44.94648 | -47.67160 |
| 0.7     | -49.786127 | -49.786838 | 60      | -43.007928 | -46.258776 |
| 0.8     | -49.786587 | -49.787521 | 70      | -38.48709 | -42.65354 |
| 0.9     | -49.787000 | -49.788186 | 80      | -33.280459 | -38.047472 |
| 1       | -49.787365 | -49.789411 | 90      | -29.978908 | -32.788581 |
| 2       | -49.788396 | -49.794511 | 100     | -26.638298 | -29.911273 |
| 3       | -49.789802 | -49.798912 | 110     | -23.180082 | -26.933141 |
| 4       | -49.776198 | -49.802825 | 120     | -19.976804 | -24.788512 |
| 5       | -49.762993 | -49.804804 | 130     | -16.860109 | -22.64152 |
| 6       | -49.745074 | -49.806567 | 140     | -13.743314 | -20.49086 |
TABLE S-VI. Energies of 3s states (meV) with different magnetic intensity \( B \) (Tesla) at temperature 0 K and 300 K for \( r_0 = 4.2086 \text{ nm}, \mu = 0.2039 \text{ m}_e, \kappa = 4.5. \)

| \( B \) (T) | 0 K | 300 K | \( B \) (T) | 0 K | 300 K |
|------------|-----|-------|------------|-----|-------|
| 0          | -16.551620 | -16.551620 | 8          | -15.001325 | -13.427883 |
| 0.1        | -16.551360 | -16.551008 | 9          | -14.204125 | -12.148735 |
| 0.2        | -16.547456 | -16.541853 | 10         | -8.618289  | -5.574895  |
| 0.3        | -16.545114 | -16.536377 | 20         | 7.125278   | 10.705982  |
| 0.4        | -16.542253 | -16.529703 | 30         | 16.266355  | 19.925459  |
| 0.5        | -16.538873 | -16.524791 | 40         | 25.946909  | 29.681931  |
| 0.6        | -16.534974 | -16.512804 | 50         | 36.044740  | 39.855984  |
| 0.7        | -16.530558 | -16.502206 | 60         | 46.477076  | 50.343774  |
| 0.8        | -16.525624 | -16.489263 | 70         | 57.184186  | 61.074853  |
| 0.9        | -16.520206 | -16.271898 | 80         | 68.124039  | 72.004863  |
| 1          | -16.514826 | -15.948198 | 90         | 79.261069  | 83.104559  |
| 2          | -16.448058 | -15.545495 | 100        | 90.569426  | 94.353023  |
| 3          | -16.320131 | -15.184186 | 110        | 102.027862 | 105.734178 |
| 4          | -15.921016 | -14.570256 | 120        | 113.619029 | 117.235016 |
| 5          | -15.654647 | -14.012804 | 130        | 125.286090 | 128.858193 |
| 6          | -15.551620 | -13.427883 | 140        | 137.140561 | 140.552814 |

ANALYSIS OF THERMO-INDUCED EFFECT BY THE PERTURBATION METHOD

In the center-of-mass frame of reference, the relative motion between the electron and hole in neutral exciton is described by the partial wave function \( \psi_K (r) \) corresponding to the pseudomomentum \( K \). This wavefunction is governed by the following one-particle Schrödinger equation

\[
\left\{ \frac{\hat{p}^2}{2\mu} + V_{RK} (r) + V_{Zeeman} (r) + V_{diamag} (r) + V_{mS} (r) - E \right\} \psi_K (r) = 0. \tag{S-49}
\]

Here, we use the Rytova-Keldysh potential

\[
V_{RK} (r) = -\frac{e^2}{8\varepsilon_0 r_0} \left[ H_0 \left( \frac{\kappa r}{r_0} \right) - Y_0 \left( \frac{\kappa r}{r_0} \right) \right] \tag{S-50}
\]

to describe the electron-hole interaction as in many Refs. [31–36]. The next two terms are the Zeeman-splitting and diamagnetic potentials, respectively,

\[
V_{Zeeman} (r) = \frac{1 - \sigma}{1 + \sigma} \frac{eB}{2\mu} l_z, \quad V_{diamag} (r) = \frac{e^2 B^2 r^2}{8\mu}, \tag{S-51}
\]

while the last term is the thermo-induced motional Stark potential

\[
V_{mS} (r) = -\sqrt{\frac{2k_B T}{M}} eB r \cos \varphi. \tag{S-52}
\]

For illustration, we show the effective potential of equation (S-49) in Fig. S-1 for two cases, with and without the thermo-induced motional Stark potential, i.e., \( T \neq 0 \) and \( T = 0 \). This figure clearly shows that at room temperature, the contribution of the added term on the effective potential is noticeable for the 2s and higher Rydberg states, and it would influence the exciton energy spectra. Now we analyze energy spectra of neutral exciton in monolayer TMDC monolayer, solving the Schrödinger equation (S-49) in the low and high limits of magnetic field intensity by the perturbation theory.
In low magnetic field intensity limit

The Schrödinger equation (S-49) without a magnetic field \((B = 0)\) is much simpler as

\[
\left\{ \frac{\hbar^2}{2\mu} + V_{RR}(r) - E^{(0)} \right\} \psi^{(0)}(r) = 0
\]

(S-53)

because there are no Zeeman-splitting, diamagnetic, and even thermo-induced motional Stark potentials. Consequently, the energy spectrum and eigenstate of neutral exciton are found as \(E^{(0)}_{nm} \) and \(\psi^{(0)}_{nm}(r) = R^{(0)}_{nm}(r)e^{im\varphi}/\sqrt{2\pi} \), respectively. Here, \(m\) is the magnetic quantum number associated with the angular momentum \(\hat{l}_z\); and \(n = n_e + |m| + 1\) is defined as the principal quantum number, with \(n_e\) being the node number of the radial wavefunction \(R^{(0)}_{nm}(r)\). At the state \(|nm\rangle\), the average separation between electron and hole is \(\langle r \rangle_{nm} = \langle R^{(0)}_{nm}(r) | r | R^{(0)}_{nm}(r) \rangle\). We note that \(E^{(0)}_{nm}(r)\) and \(R^{(0)}_{nm}(r)\) are obtained by numerical calculation, particularly by the method described in Sec.

Turning on the magnetic field \((B > 0)\) such that its typical length is much larger than the average exciton radius, \(l_B = \sqrt{\hbar/eB} \gg \langle r \rangle_{nm}\), all the Zeeman-splitting, diamagnetic, and thermo-induced motional Stark potentials can be treated as perturbed interactions besides the zeroth-order Hamiltonian in Eq. (S-53). Both the Zeeman-splitting and diamagnetic potentials contribute to the first-order correction via Zeeman-splitting and diamagnetic energies

\[
\left\langle \psi^{(0)}_{nm} \right| V_{Zeeman} \left| \psi^{(0)}_{nm} \right\rangle = \frac{1 - \sigma \hbar m}{1 + \sigma \hbar m} eB,
\]

(S-54)

\[
\left\langle \psi^{(0)}_{nm} \right| V_{diamag} \left| \psi^{(0)}_{nm} \right\rangle = \frac{c^2B^2}{8\mu} \langle r^2 \rangle_{nm}.
\]

(S-55)

Since the original state \(\psi^{(0)}_{nm}(r)\) exhibits the \(SO(2)\) symmetry of neutral exciton and the thermo-induced motional Stark potential \(V_{mS}(r)\) is proportional to \(r \cos \varphi\), its first-order correction must vanish

\[
\left\langle \psi^{(0)}_{nm} \right| V_{mS} \left| \psi^{(0)}_{nm} \right\rangle = 0.
\]

(S-56)

However, the thermo-induced motional Stark effect solely appears in the second-order correction of energy as

\[
\sum_{\langle n'm' \rangle \neq \langle nm \rangle} \left| \left\langle \psi^{(0)}_{nm} \right| V_{mS} \left| \psi^{(0)}_{n'm'} \right\rangle \right|^2 = -\alpha_{nm} \frac{k_B T}{M} c^2 B^2.
\]

(S-57)

Here, \(\alpha_{nm}\) is the zero-field polarizability of the exciton

\[
\alpha_{nm} = -\sum_{n' \geq |m'| + 1, m' = m \pm 1} \int_0^{+\infty} R^{(0)\ast}_{nm}(r) R^{(0)}_{n'm}(r) r^2 dr \frac{E^{(0)}_{nm} - E^{(0)}_{n'm'}}{E^{(0)}_{nm} - E^{(0)}_{n'm'}}.
\]

(S-58)

Finally, the energy of magnetoe exciton at the state \(|nm\rangle\) is obtained as

\[
E^{(2)}_{nm}(B,T) \approx E^{(0)}_{nm} + \frac{1 - \sigma \hbar m}{1 + \sigma \hbar m} eB + \frac{c^2B^2}{8\mu} \langle r^2 \rangle_{nm} - \alpha_{nm} \frac{k_B T}{M} e^2 B^2.
\]

(S-59)

This is the equation (4) in the main text. In other words, the quadratic thermo-induced motional Stark correction in the low magnetic field is proportional to the square of magnetic field strength

\[
\Delta E_{nm}(B,T) = E^{(2)}_{nm}(B,T) - E_{nm}(B,0) \approx \alpha_{nm} \frac{k_B T}{M} e^2 B^2.
\]

(S-60)

From energies of the states 1s, 2s, 3s, 2p−1, and 2p+1 in Tables S-II, S-III, S-IV, S-V, and S-VI, the quadratic thermo-induced motional Stark corrections in the low magnetic field \(\Delta E_{nm}(B,T)\) for these states are numerically determined. Consequently, the zero-field polarizability of exciton \(\alpha_{nm}\) and the thermo-induced Stark correction on
diamagnetic coefficient $\Delta \sigma_{nm} = -\frac{2}{\hbar^2} \alpha_{nm} k_B T$ are revealed by fitting the data of $\Delta E_{nm}(B, T)$ versus $B^2$ in Eq. (S-60). These results are presented in Table 2 of the main text.

Figure S-2 indicates that the quadratic thermo-induced motional Stark corrections of $1s$, $2s$, $3s$, $2p_{-1}$, and $2p_{+1}$ states depend on $B^2$ for the low magnetic field regime.

\[ \Delta E_{nm}(B, T) \text{ versus } B^2 \]

![Figure S-2](image-url)  
**FIG. S-2.** The dependence of quadratic thermo-induced motional Stark corrections $\Delta E_{nm}(B, T)$ for various states: $1s$ (black), $2s$ (red), $3s$ (blue), $2p_{-1}$ (blue dashed), and $2p_{+1}$ (blue dot-dashed) on magnetic field strength $B$ for the low magnetic field regime.

**In high magnetic field intensity limit**

Suppose the magnetic field is so large that its typical length is much smaller than the average exciton radius, $l_B \ll \langle r \rangle$, the diamagnetic potential $V_{\text{diamag}} = \frac{e^2 B^2}{8\mu} r^2$ (the harmonic oscillator potential of frequency $\omega_B = eB/2\mu$) becomes dominant. In this case, the energy spectrum tends to the conventional Landau levels. Within the effect of Zeeman-splitting potential $V_{\text{Zeeman}}$, these zero-temperature Landau levels are shifted as

\[ E_{nm}^{(0)}(B \to \infty, T = 0) = \frac{\hbar}{2\mu} \left( 2n - |m| - 1 + \frac{1 - \sigma}{1 + \sigma} m \right) eB, \]

and the corresponding eigenstate is of the isotropic harmonic oscillator with the wave function

\[ \psi_{nm}^{(0)}(r) = \frac{1}{l_B R_{nm}^{(0)}} \left( \frac{r^2}{l_B^2} \right)^\frac{1}{4} e^{im\varphi} \frac{e^{i2\pi n}}{\sqrt{2^n}}, \]

where $R_{nm}^{(0)}$ is the dimensionless radial wave function of the dimensionless variable $r^2/l_B^2$.

Similar to the low magnetic field limit in the finite temperature, the thermo-induced motional Stark potential in the high magnetic field limit contributes to the second-order correction in the perturbation theory as

\[ \sum_{(n', m') \neq (n, m)} \frac{\left| \langle \psi_{nm}^{(0)} | V_{nm} S | \psi_{n'm'}^{(0)} \rangle \right|^2}{E_{nm}^{(0)} - E_{n'm'}^{(0)}}. \]

It results in the energy spectrum of magnetoexciton behaving as

\[ E_{nm}^{(2)}(B, T) \approx \frac{\hbar}{2\mu} \left( 2n - |m| - 1 + \frac{1 - \sigma}{1 + \sigma} m \right) eB - \frac{8\mu \beta_{nm}}{M} k_B T, \]

(S-64)
where \( \beta_{nm} \) is a dimensionless constant calculated as

\[
\beta_{nm} = -\frac{e^2 B^2}{4\mu} \sum_{(n',m') \neq (n,m)} \left| \frac{\langle \psi_{nm}^{(0)} | r \cos \varphi | \psi_{n'm'}^{(0)} \rangle}{E_{nm}^{(0)} - E_{n'm'}^{(0)}} \right|^2
\]

\[
= -\sum_{n' \geq |m'|+1} \sum_{m'=m \pm 1} \frac{1}{2(n-n')} \int_{0}^{+\infty} R_{nm}^{(0)}(x) R_{n'm'}^{(0)}(x) \sqrt{x} dx \frac{1}{n-n'} \left( [m] - [m'] + \frac{1-\sigma}{1+\sigma} (m - m') \right). \tag{S-65}
\]

Therefore, the quadratic thermo-induced motional Stark correction in the high magnetic field limit solely depends on temperature as

\[
\Delta E_{nm}(B, T) = E_{nm}^{(2)}(B, T) - E_{nm}(B, 0) \approx -\frac{8\mu \beta_{nm}}{M} k_B T. \tag{S-66}
\]

Although these calculations are only valid for extremely high magnetic intensity, the magnetic independence of \( \Delta E_{nm}(B, T) \) can still be observed in our numerical calculations. Figure S-3 below illustrates how the quadratic thermo-induced motional Stark correction \( \Delta E_{nm}(B, T) \) constantly behaves in the high magnetic field regime.

**FIG. S-3.** The dependence of quadratic thermo-induced motional Stark correction \( \Delta E_{nm}(B, T) \) for various states: 1s (black), 2s (red), 3s (blue), 2p_{-1} (blue dashed), and 2p_{+1} (blue dot-dashed) on magnetic field strength \( B \) for the high magnetic field regime.

**Thermo-induced deformation of magnetoexciton wave functions by symmetry-breaking mechanism**

The influence of thermo-induced motional Stark potential on the wave function of magnetoexciton is also important because this potential breaks the \( SO(2) \) symmetry of magnetoexciton. Indeed, the angular momentum \( \hat{l}_z \) is no longer conserved when we turn on the thermo-induced motional Stark potential. Hence, we can witness the deformation of magnetoexciton’s orbital from this breaking symmetry mechanism.

In detail, the relative Hamiltonian of electron-hole pair under the presence of the thermo-induced motional Stark potential reads

\[
\hat{H}_{rel}(T) = \hat{H}_{rel}(0) + V_{mS}(r), \tag{S-67}
\]
where the zero-temperature relative Hamiltonian is given as
\[ H_{rel}(0) = \frac{1}{2\mu} \hat{p}^2 + \frac{1 - \sigma eB}{1 + \sigma} \hat{l}_z + \frac{e^2 B^2}{8\mu} r^2 + V_{RK}(r) \]
\[ = -\frac{\hbar^2}{2\mu} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \right) \right] + \frac{l_z^2}{2\mu} + \frac{1 - \sigma eB}{1 + \sigma} \hat{l}_z + \frac{e^2 B^2}{8\mu} r^2 + V_{RK}(r). \] (S-68)

One can easily verify that each term of the zero-temperature relative Hamiltonian (S-68) commutes with the relative angular momentum \( \hat{l}_z = -i\hbar \partial / \partial \phi \). The first, fourth, and fifth terms in Eq. (S-68) commute with \( \hat{l}_z \) because they only depend on the radial variable \( r \) and do not depend on the angle variable \( \phi \). On the other hand, the second and third terms are polynomials of \( \hat{l}_z \) by themselves and trivially commute with \( \hat{l}_z \). Then
\[ [\hat{l}_z, H_{rel}(0)] = 0, \] (S-69)
i.e., the angular momentum \( \hat{l}_z \) is conserved at zero temperature \( T = 0 \). In other words, the magnetoexciton at zero temperature exhibits the \( SO(2) \) symmetry. A direct consequence of this \( SO(2) \) symmetry is that the wavefunction of the relative motion of magnetoexciton must be in the following form
\[ \psi_{nm}^{(0)}(r) = R_{nm}^{(0)}(r) \frac{e^{im\phi}}{\sqrt{2\pi}}, \] (S-70)
where its modulus does not depend on the angle variable \( \phi \):
\[ |\psi_{nm}^{(0)}(r)|^2 = \left|R_{nm}^{(0)}(r)\right|^2. \] (S-71)

We say that magnetoexciton at zero temperature has circular orbitals.

The scenario changes when we turn on the temperature \( T \neq 0 \). Including the thermo-induced motional Stark potential \( V_{mS}(r) = -\frac{2k_B T}{M} eB r \cos \phi \), makes the angular momentum \( \hat{l}_z \) no longer commutes with the Hamiltonian
\[ [\hat{l}_z, H_{rel}(T)] = [\hat{l}_z, H_{rel}(0)] + [\hat{l}_z, V_{mS}(r)] \]
\[ = -i\hbar \frac{\partial}{\partial \phi} - \sqrt{\frac{2k_B T}{M}} eB r \cos \phi \]
\[ = -i\hbar \sqrt{\frac{2k_B T}{M}} eB r \sin \phi \neq 0. \] (S-72)

We say that the thermo-induced motional Stark potential breaks the \( SO(2) \) symmetry of magnetoexciton. Therefore, it is expected that the thermo-induced motional Stark effect could deform the magnetoexciton’s orbitals and change the average distance of the electron-hole pair. We consider the zero-temperature wave functions of magnetoexciton as zeroth-order Hamiltonian and then treat the thermo-induced motional Stark potential as a perturbation term. The zeroth-order Schrödinger equation for magnetoexciton reads
\[ \left\{ \frac{\hat{p}^2}{2\mu} + V_{RK}(r) + V_{Zeeman}(r) + V_{diamag}(r) - E^{(0)}(r) \right\} \psi^{(0)}_{K}(r) = 0. \] (S-73)

The energy spectrum and eigenstates of magnetoexciton are \( E_{nm}^{(0)} \) and \( \psi_{nm}^{(0)}(r) = R_{nm}^{(0)}(r) \frac{e^{im\phi}}{\sqrt{2\pi}} \), respectively.

Taking into account the first-order correction caused by this thermo-induced motional Stark potential, we obtain the temperature-dependent wave functions of magnetoexciton as
\[ \psi_{nm}^{T}(r) \approx R_{nm}^{(0)}(r) \frac{e^{im\phi}}{\sqrt{2\pi}} \sqrt{\frac{2k_B T}{M}} eB \sum_{n' \geq |m|+1} f_{nm;n',m+1} R_{n',m+1}^{(0)}(r) \frac{e^{i(m+1)\phi}}{\sqrt{2\pi}} - \sqrt{\frac{2k_B T}{M}} eB \sum_{n' \geq |m-1|+1} f_{nm;n',m-1} R_{n',m-1}^{(0)}(r) \frac{e^{i(m-1)\phi}}{\sqrt{2\pi}}, \] (S-74)
where the coefficients \( f_{nm;n'm'} \) are given by the following integrals
\[ f_{nm;n'm'} = \int_{0}^{+\infty} R_{nm}^{(0)}(r) R_{n'm'}^{(0)}(r) r^2 dr \frac{E_{nm}^{(0)} - E_{n'm'}^{(0)}}{E_{nm}^{(0)} - E_{n'm'}^{(0)}}. \] (S-75)
As a result, the orbital of magnetoexciton is deformed along the $Ox$ axis because the probability density is no longer angle-independent

$$
|\psi_{nm}(r)|^2 = \frac{1}{2\pi} \left| R_{nm}^{(0)}(r) \right|^2 - \frac{1}{2\pi} \sqrt{\frac{2k_B T}{M}} e^B \sum_{n'} \left( f_{nm;n',m+1} R_{nm}^{(0)}(r) R_{n',m+1}^{(0)}(r) e^{i\varphi} + f_{nm;n',m-1} R_{nm}^{(0)}(r) R_{n',m-1}^{(0)}(r) e^{-i\varphi} + c.c \right) \\
+ \frac{1}{2\pi} \sqrt{\frac{2k_B T}{M}} e^B \sum_{n',n''} \left[ f_{nm;n',m+1} f_{nm;n'',m+1} R_{n',m+1}^{(0)*} R_{n'',m+1}^{(0)}(r) \right] \\
+ \frac{1}{2\pi} \sqrt{\frac{2k_B T}{M}} e^B \sum_{n',n''} \left[ f_{nm;n',m-1} f_{nm;n'',m-1} R_{n',m-1}^{(0)*} R_{n'',m-1}^{(0)}(r) \right] \\
+ \left( f_{nm;n',m+1} f_{nm;n'',m+1} R_{n',m+1}^{(0)*} R_{n'',m+1}^{(0)}(r) e^{-2i\varphi} + c.c \right) .
$$

(S-76)

The symmetry breaking is clear in the squared modulus of the wave functions $|\psi|^2$ of 2s, 3s, 2p₁ and 2p₂ states at temperatures of 0K and 300K, as shown in Fig. S-4. The effect is also seen in the orbital of the 1s state but is very slight.

![FIG. S-4. Squared modulus of wavefunction $|\Psi|^2$ as a function of electron-hole separation $r$ along $x$ and $y$ axis for different states.](image)

A direct consequence of the orbital’s deformation is the change of the average separation between electron and hole in magnetoexcitons

$$
\langle r \rangle_{nm} = \int_{-\infty}^{+\infty} \int_{0}^{2\pi} \left| \psi_{nm}(r) \right|^2 r^2 dr d\varphi \\
= \int_{0}^{+\infty} \left| R_{nm}^{(0)}(r) \right|^2 r^2 dr + \frac{2k_B T}{M} e^B \sum_{n',n''} f_{nm;n',m} f_{nm;n'',m} \int_{0}^{+\infty} R_{n',m'}^{(0)*} R_{n'',m'}^{(0)}(r) r^2 dr \\
= \langle r \rangle_{nm} + \gamma_{nm} e^B \frac{2k_B T}{M} ,
$$

(S-77)

with

$$
\gamma_{nm} = \sum_{n',n'' \geq |m'| + 1} f_{nm;n',m} f_{nm;n'',m} \int_{0}^{+\infty} R_{n',m'}^{(0)*} R_{n'',m'}^{(0)}(r) r^2 dr .
$$

(S-78)
Figure S-5 shows how the average electron-hole separation $<r>$ depends on the magnetic field at zero and room temperatures. As seen in the small panels, the change $\Delta <r>$ is proportional to $B^2$ for the low magnetic field limit, as predicted by the perturbation theory.

**FIG. S-5.** Magnetic field dependence of average radius $\langle r \rangle$ of magnetoexciton with different states. Small panels show the change of average radius $\Delta \langle r \rangle$ by temperature.

**Squared modulus of magnetoexciton wave functions at zero separation of electron-hole pair for np and nd states**

According to Elliot formula (see equation (9) in the main text), the signal of exciton peaks on the absorption spectra mainly depends on the oscillation strength, which is proportional to the squared modulus of the wave function $|\psi_{nm}(r = 0)|^2$ at zero distance of the electron-hole pair.

At zero temperature $T = 0$, the conservation of the angular momentum $\hat{l}_z$, i.e., the $SO(2)$ symmetry of Schrödinger equation (S-73), suggests the form of the radial wave function as follows

$$R_{nm}^{(0)} \propto r^{|m|}e^{-f(r)}u(r).$$  \hfill (S-79)

Therefore, except for the $s$-states, the wave function at zero distance $r = 0$ for all other states must vanish

$$\left|\psi_{np}^{(0)}(r = 0)\right|^2 = \left|\psi_{nd}^{(0)}(r = 0)\right|^2 = \ldots = 0.$$  \hfill (S-80)

When we turn on the temperature ($T \neq 0$), the orbital of magnetoexciton is deformed, as in Eq. (S-76) based on the perturbation theory calculations. Hence, for $p$-states, the squared modulus becomes non-vanished

$$\left|\psi_{np}^{T}(r = 0)\right|^2 = \frac{2k_BT}{M}e^2B^2\sum_{n',n''} f_{np; n''s}^* f_{np; n's} \psi_{n''s}^{(0)*}(r = 0)\psi_{n's}^{(0)}(r = 0) \propto \frac{k_BT}{M}.$$  \hfill (S-81)

Nonzero wavefunction at zero e-h separation is witnessed for $2p_{\pm 1}$ states as shown in small panels in Fig. S-4. This circumstance leads to the emergence of the $p$-state peaks on the absorption spectra of neutral magnetoexciton, as shown in Fig. 4 of the main text and more details in Fig. S-6.
Our numerical results also highlight the emergence of the $d$-state peaks on the neutral magnetoexciton’s absorption spectra. To explain this emergence, we need a higher-order correction beyond the quadratic thermo-induced motional Stark effect. Skipping the detailed calculations, we obtain the squared modulus of magnetoexciton wave function at zero separation for the $d$-state, which is proportional to the temperature square as
\[
|\psi_{nd}(r = 0)|^2 \propto \left( \frac{k_B T}{M} \right)^2.
\]
Thus, the intensity of $d$-states peaks is much smaller than that of the $p$-states.

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