Magnetoeexcitons in phosphorene monolayers, bilayers, and van der Waals heterostructures

Roman Ya. Kezerashvili$^{1,2}$ and Anastasia Spiridonova$^{1,2}$

$^1$New York City College of Technology, The City University of New York, Brooklyn, NY 11201, USA
$^2$The Graduate School and University Center, The City University of New York, New York, NY 10016, USA

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We study direct and indirect excitons in Rydberg states in phosphorene monolayers, bilayer and van der Waals (vdW) heterostructure in an external magnetic field, applied perpendicular to the monolayer or heterostructure within the framework of the effective mass approximation. Binding energies of magnetoeexcitons are calculated by a numerical integration of the Schrödinger equation using the Rytova-Keldysh potential for direct magnetoeexcitons and both the Rytova-Keldysh and Coulomb potentials for indirect one. The latter allows to understand the role of screening in phosphorene. We report the magnetic field energy contribution to the binding energies and diamagnetic coefficients (DMCs) for magnetoeexcitons that strongly depend on the effective mass of electron and hole and their anisotropy and can be tuned by the external magnetic field. We demonstrate theoretically that the vDW phosphorene heterostructure is a novel category of 2D semiconductor offering a tunability of the binding energies of magnetoeexcitons by mean of external magnetic field and control the binding energies and DMCs by the number of hBN layers separated two phosphorene sheets. Such tunability is potentially useful for the devices design.

I. INTRODUCTION

The most recent addition to the growing family of 2D material is phosphorene that is the monolayer of black phosphorus (BP). The BP is composed of individual phosphorene layers. The blossoming interest in phosphorene derives partially from its direct gap that is retained in both monolayer and bulk structure, high mobility, and high on-off current ratio in field-effective transistors [1,4]. In contrast, these characteristics simultaneously are not present in graphene, transitional metal dichalcogenides (TMDCs): WS$_2$, WSe$_2$, MoS$_2$, MoSe$_2$, or Xenes: silicene, germanene, stanene, making phosphorene a promising material for electronic and optical applications. Black phosphorus is the most stable of phosphorus allotropes. It was first synthesized in 1914 by Bridgman [5]. While bulk black phosphorus has interesting properties and was extensively studied in twentieth century [6–11], it was not used in the design of electronic devices.

However, everything has changed after the discovery of graphene in 2004 [12] which paved the way for two-dimensional materials. Initially, the research was focused on graphene [13, 14] and TMDCs [15–23] then silicene, germanene, stanene, making phosphorene a promising material for electronic and optical applications. Black phosphorus has high mobility and on-off ratio but a lack of a gap impedes its use in the design of electronic devises [2, 4]. TMDCs have a gap [28–30], but its carrier mobility is orders of magnitudes lower than in graphene. The phosphorene that has been synthesized in 2014 has advantages over graphene, TMDCs, and Xenes. Its most remarkable properties include thickness-dependent band gap, strong in-plane anisotropy, and high carrier mobility.

BP has a structure where monolayer appears to be composed of two distinct planes made of puckered honeycomb structure [31–33]. This results in an anisotropic electronic structure. Due to phosphorene unique topological structure and differences between the armchair (AC) and zigzag (ZZ) directions, it displays strong in-plane anisotropy. Many properties of phosphorene in these two principal directions are drastically different. The anisotropic structure is strongly reflected in effective masses of charge carriers and leads to anisotropic effective masses of electrons and holes along AC and ZZ (x and y) directions. Along the AC direction the effective electron and hole masses are smaller than along the ZZ direction [9, 31–33]. The distinct features of BP is that the direct gap located at the Γ point is preserved in the monolayer and bulk structure. This material is a direct band gap semiconductor with a strongly anisotropic dispersion in the vicinity of the gap. It is worth noting that the unusual structure of phosphorene sets it aside from graphene and other widely studied 2D semiconductors.

Since the synthesis of phosphorene, it has been extensively studied. For example, optical and thermal properties have been considered in Refs. [33–37], in plane electric field has been studied in Refs. [38–41], the effects of the strain on different properties of phosphorene have been addressed in Refs. [42–44], the Landau levels have been reported in Refs. [45–50].

Phosphorene hosts tightly bound excitons [31, 51–54]. Similarly to other monolayer semiconductors, reduced dimensionality and reduced screening of the Coulomb attraction lead to a high exciton binding energy in phosphorene. Moreover, the exciton binding energy in phosphorene is larger than the one in other 2D materials. Excitons in semiconductors in the presence of the external magnetic field have been studied for the past sixty years. Elliot and Loudon [55] and Hasegawa and Howard [56] developed the theory of the Mott exciton in the strong magnetic field.
Authors in Refs. [57–59] addressed Mott excitons. Excitons in TMDCs monolayers, bilayer, and the double-layer heterostructure in the presence of the external magnetic field have been extensively studied. The diamagnetic shifts have been reported in Refs. [23, 60–67], and Zeeman shifts have been reported in Refs. [68–73]. We cite these works, but the recent literature on the subject is not limited by them. However, there is a lack of similar research on excitons in phosphorene. This motivates us to study the effect of the external magnetic field on the binding energies of Rydberg states of magnetoeexcitons in monolayer, bilayer, and the double-layer heterostructure composed of phosphorene and to calculate diamagnetic coefficients (DMCs).

In this paper, we study the dependence of the magnetoe exciton binding energy of Rydberg states: 1s, 2s, 3s, and 4s, on the external magnetic field perpendicular to a monolayer or heterostructure that is varied between 0 and 60 T and report the diamagnetic coefficients (i) for the direct magnetoe excitons in a freestanding (FS) and encapsulated phosphorene monolayers, (ii) for the indirect magnetoe exciton in bilayer composed of two phosphorene monolayers, (iii) for the indirect magnetoe excitons in heterostructure formed by two phosphorene monolayers and separated by N hBN monolayers. The latter van der Waals heterostructure is denoted as vdW. In our approach, we numerically solve the Schrödinger equation for the magnetoe exciton and obtain eigenfunctions and eigenvalues. Then we obtain the energy contribution from the magnetic field to the binding energies and use it to calculate diamagnetic coefficients. For the direct exciton, we solve the Schrödinger equation with the Rytova-Keldysh potential [74, 75], and for the indirect exciton, we solve the Schrödinger equation with the Rytova-Keldysh and the Coulomb potentials to understand the role of the screening in phosphorene.

The remainder of this paper is organized in the following way. In section II the theoretical model for the description of an electron-hole system in the external magnetic field with the charge carriers effective mass anisotropy is presented. Results of calculations of binding energies of Rydberg states and DMCs for direct magnetoe excitons in a freestanding and encapsulated phosphorene and indirect magnetoe excitons in FS bilayer and vdW phosphorene heterostructures are presented in Sec. III. Finally, conclusions follow in Sec. IV.

II. THEORETICAL MODEL

It is known that electrostatically-bound electrons and holes in the external magnetic field form magnetoe excitons. In this section, following Refs. [23, 27, 58, 67], we introduce briefly the theoretical model for the description of the Mott-Wannier magnetoe exciton in phosphorene. We consider the energy contribution from the external magnetic field to the Rydberg states binding energies of magnetoe excitons and diamagnetic coefficients (DMCs). In the system under consideration, excitons are confined in a 2D freestanding and encapsulated phosphorene monolayer, FS bilayer phosphorene and van der Waals heterostructure, where N layers of hBN monolayers separate two phosphorene monolayers. In the latter two cases equal number of electrons and holes are located in parallel phosphorene monolayers at a distance D away. The corresponding schematic illustrations of these systems are shown in Fig. 1.

It is worth mentioning that we are considering the monolayers of hBN as an insulator. Phosphorene encapsulated between hBN layers is robust to oxidation and exhibits high mobilities. Moreover, hBN also has a high dielectric constant, resulting in a strong damping of the electrostatic repulsion by charged impurities which are responsible for the decrease of carriers mobility.

Let us introduce the coordinate vectors of the electron and hole for the Mott-Wannier exciton in the phosphorene layer. The following in-plane coordinates \( \mathbf{r}_1 = (x_1, y_1) \) and \( \mathbf{r}_2 = (x_2, y_2) \) for an electron and hole, respectively, will be used in our description. We assume that at low momentum \( \mathbf{p} = (p_x, p_y) \), i.e., near the \( \Gamma \) point, the single electron and hole energy spectrum \( \varepsilon_l^{(0)}(\mathbf{p}) \) is given by

\[
\varepsilon_l^{(0)}(\mathbf{p}) = \frac{p_x^2}{2m_x} + \frac{p_y^2}{2m_y}, \quad l = e, h,
\]

where \( m_x \) and \( m_y \) are the electron and hole effective masses along the \( x \) and \( y \) directions, respectively. We assume that \( OX \) and \( OY \) axes correspond to the armchair and zigzag directions in a phosphorene monolayer, respectively.

The anisotropic nature of the 2D phosphorene atomic semiconductor, in contrary to other 2D isotropic materials such as graphene and TMDC semiconductors, breaks the central symmetry and requires for the description of excitons the use of the Cartesian coordinates. The asymmetry of the electron and hole dispersion in phosphorene is reflected in the Hamiltonian for the Mott-Wannier magnetoe exciton, and within the framework of the effective mass approximation
the Hamiltonian for an interacting electron-hole pair in phosphorene in the external magnetic field reads ($\hbar = c = 1$)

$$
\hat{H} = \frac{1}{2m_e^x}(i\nabla_{x_e} - eA_x(r_e))^2 + \frac{1}{2m_e^y}(i\nabla_{y_e} - eA_y(r_e))^2 + \frac{1}{2m_h^x}(i\nabla_{x_h} + eA_x(r_h))^2 + \frac{1}{2m_h^y}(i\nabla_{y_h} + eA_y(r_h))^2 + V(|r_e - r_h|),
$$

(2)

where the $m_j^i$, $i = e, h$ correspond to the effective mass of the electron or hole in the $x$ or $y$ direction, respectively, and $V(|r_e - r_h|)$ describes the electrostatic interaction between the electron and hole. When the electron and hole are located in 2D plane, we use the Rytova-Keldysh (RK) potential $\chi_{2D}$ that is widely used for the description of charge carriers interaction in 2D materials. The RK potential is a central potential, and the interaction between the electron and hole for direct excitons in a monolayer has the form $\chi_{2D}$:

$$
V_{RR}(r) = -\frac{\pi k e^2}{2\kappa \rho_0} \left[ H_0 \left( \frac{r}{\rho_0} \right) - Y_0 \left( \frac{r}{\rho_0} \right) \right],
$$

(3)

where $r = r_e - r_h$ is the relative coordinate between the electron and hole. In Eq. (3), $e$ is the charge of the electron, $\kappa = (\epsilon_1 + \epsilon_2)/2$ describes the surrounding dielectric environment, $\epsilon_1$ and $\epsilon_2$ are the dielectric constants below and above the monolayer, $H_0$ and $Y_0$ are the Struve and Bessel functions of the second kind, respectively, and $\rho_0$ is the screening length. The screening length $\rho_0$ can be written as $\rho_0 = 2\pi \chi_{2D}/\kappa$, where $\chi_{2D}$ is the 2D polarizability, which in turn is given in $\chi_{2D}$. At the long-range distances $V_{RR}$ retains $1/r$ behavior as the Coulomb potential, for smaller distances the potential well is logarithmic.

Following the standard procedure $\chi_{2D}$ for the separation of the relative motion of the electron-hole pair from their center-of-mass motion one introduces variables for the center-of-mass of an electron-hole pair $R = (X, Y)$ and the relative motion of an electron and a hole $r = (x, y)$, as $X = (m_e^x x_1 + m_h^x x_2)/(m_e^x + m_h^x)$, $Y = (m_e^y y_1 + m_h^y y_2)/(m_e^y + m_h^y)$, $x = x_1 - x_2$, $y = y_1 - y_2$, $r^2 = x^2 + y^2$. The Schrödinger equation with Hamiltonian (2) has the form $H\Psi(R_1, R_2) = \mathcal{E}\Psi(R_1, R_2)$, where $\Psi(R_1, R_2)$ and $\mathcal{E}$ are the eigenfunction and eigenenergy, respectively. One can write $\Psi(R_1, R_2)$ in the form $\Psi(R_1, R_2) = \Phi(R, r) = e^{i\mathbf{P}R/\hbar}\Phi(x, y)$, where $\mathbf{P} = (P_x, P_y)$ is the momentum of the center-of-mass of the electron-hole pair and $\Phi(x, y)$ is the wave function of the relative motion of the electron-hole pair. Following Refs. $\chi_{2D}$, after lengthy calculations one obtains the equation that describes the Mott–Wannier exciton in Rydberg optical states in the external magnetic field perpendicular to the phosphorene monolayer. Finally, the equation for

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FIG. 1. (Color online) Schematic illustration of magnetoexcitons in phosphorene monolayers and heterostructures. (a) A direct magnetoexciton in a freestanding phosphorene monolayer. (b) A direct magnetoexciton in an encapsulated phosphorene monolayer. (c) An indirect magnetoexciton in a freestanding bilayer phosphorene heterostructure. (d) An indirect magnetoexciton in phosphorene van der Waals heterostructure.
the relative motion of the electron and hole in the phosphorene monolayer with zero center-of-mass momentum reads

\[
\left[-\frac{1}{2\mu_x} \frac{\partial^2}{\partial x^2} - \frac{1}{2\mu_y} \frac{\partial^2}{\partial y^2} + \frac{e^2}{8\mu_x} B^2 x^2 + \frac{e^2}{8\mu_y} B^2 y^2 + V(x, y)\right] \Phi(x, y) = E \Phi(x, y),
\]

where \(\mu_x = \frac{m_e^2 m_h^b}{m_e^2 + m_h^b}\) and \(\mu_y = \frac{m_e^a m_h^b}{m_e^a + m_h^b}\) are the reduced masses, related to the relative motion of an electron-hole pair in the \(x\) and \(y\) directions, respectively. In Eq. (4) the anisotropy is present in the kinetic and magnetic terms, while the potential term has isotropic form.

Following Refs. [79, 80] one can obtain from (4) the expectation value for the ground state energy. For the case of \(V_{RK}(x, y)\) potential we have

\[
E = \left\langle -\frac{1}{2\mu_x} \frac{\partial^2}{\partial x^2} \right\rangle + \left\langle -\frac{1}{2\mu_y} \frac{\partial^2}{\partial y^2} \right\rangle + \left\langle \frac{e^2}{8\mu_x} B^2 x^2 \right\rangle + \left\langle \frac{e^2}{8\mu_y} B^2 y^2 \right\rangle + \left\langle V_{RK}(x, y) \right\rangle.
\]

The later expression could be viewed as the sum of the average values of the operators of kinetic and potential energies in 2D space obtained by using the corresponding eigenfunction \(\Phi(x, y)\) of the exciton. Phosphorene exhibits charge carriers effective mass anisotropy with lighter effective masses along the armchair direction and heavier effective masses along the zigzag direction that leads to the reduced mass anisotropy: \(\mu_y > \mu_x\). For the set of masses presented in Table I the ratio \(\mu_y/\mu_x\) varies from \(\sim 7\) to \(16\). Therefore, from the latter expression one can conclude that contributions from the kinetic and magnetic energies to the total ground state energy can be by the order of magnitude different for AC and ZZ directions. In particular, the kinetic energy along the AC direction is much larger than that along the ZZ direction.

Thus, the anisotropic nature of the 2D phosphorene atomic semiconductors, in contrast to other 2D materials such as graphene, Xenes, and TMDC semiconductors, allows excitons to be confined in a quasi-one-dimensional space predicted in theory [1, 81], leading to remarkable phenomena arising from the reduced dimensionality and screening. In Fig. 2 the total potential \(W(x, y) = V_{RK}(x, y) + \frac{e^2}{8\mu_x} B^2 x^2 + \frac{e^2}{8\mu_y} B^2 y^2\) that acts on the electron-hole system in phosphorene is presented. One can observe the anisotropic structure of this potential and its asymmetry with respect to the AC and ZZ directions.

Let us now consider the indirect magnetoexcitons formed by electrons and holes located in two different phosphorene monolayers in the bilayer or vdW heterostructure. In the latter case the phosphorene layers are separated by \(N\) layers of hBN monolayers. Such magnetoexcitons have a longer lifetime than the direct excitons due to longer recombination time. Equation (4) still describes the indirect exciton. However, for indirect excitons, the expressions for the interaction between the electron and hole in Eq. (4) can be written as:

\[
V_{RK}(\sqrt{\rho^2 + D^2}) = -\frac{\pi ke^2}{2\kappa \rho_0} \left[ H_0 \left( \frac{\sqrt{\rho^2 + D^2}}{\rho_0} \right) - Y_0 \left( \frac{\sqrt{\rho^2 + D^2}}{\rho_0} \right) \right],
\]

for the RK potential, and

\[
V_C \left( \sqrt{\rho^2 + D^2} \right) = -\frac{ke^2}{\kappa} \left( \frac{\sqrt{\rho^2 + D^2}}{\rho_0} \right)
\]

for the Coulomb potential and where \(\rho^2 = x^2 + y^2\). Equations (5) and (6) describe the interaction between the electron and hole that are located in different parallel phosphorene monolayers separated by a distance \(D = h + Nh_{\text{hBN}}\), where \(h_{\text{hBN}} = 0.333\) nm is the thickness of the hBN layer and \(h\) is the phosphorene thickness given in Table I. Therefore, one can obtain the eigenfunctions and eigenenergies of magnetoexcitons by solving Eq. (4) using the potential (5) \(V_{RK}\) for direct magnetoexcitons, or using either potential (5) \(V_{RK}\) or (6) \(V_C\) for indirect magnetoexcitons.

### Table I. Parameters for phosphorene.

Four sets of reduced masses for phosphorene that are used in calculations as input parameters. The anisotropic reduced masses \(\mu_x\) and \(\mu_y\) are obtained based on effective masses of the electron and hole given in Ref. [82] for the set 1, in Ref. [83] for the set 2, in Ref. [84] for the set 3, and in Ref. [1] for the set 4. \(\mu_x\) and \(\mu_y\) are in units of the electron mass, \(m_0\). \(\chi_{2D}\) and \(h\) are the polarizability and thickness of phosphorene, respectively, in nm.

| \(\mu_x\) | \(\mu_y\) | \(\mu_y/\mu_x\) | \(\chi_{2D}\) (nm) | \(h\) (nm) |
|-----|-----|-----|-------|-------|
| set 1 | 0.06296 | 0.96774 | 15.37 | 0.41 \(^a\) |
| set 2 | 0.06667 | 0.88780 | 13.32 | 0.541 \(^b\) |
| set 3 | 0.09122 | 0.6599 | 7.23 | |
| set 4 | 0.07969 | 0.9498 | 11.92 | |

\(^a\) Reference [85].

\(^b\) Reference [86].
III. RESULTS OF CALCULATIONS AND DISCUSSION

We report the dependence of the energy contribution from the external magnetic field to the binding energies of magnetoexcitons in Rydberg states $1s$, $2s$, $3s$, and $4s$ in the FS (Fig. 1(a)) and encapsulated by hBN (Fig. 1(b)) phosphorene, the FS phosphorene bilayer (Fig. 1(c)), and the vdW heterostructure (Fig. 1(d)) on the magnetic field. The diamagnetic coefficients for the monolayers, bilayer, and vdW phosphorene heterostructure are reported for the first time.

In calculations, we use effective masses for electron and hole found in literature Refs. [1, 82–84], which are obtained by using the first principle calculations. The lattice constants in Refs. [1, 82–84] do not coincide with each other and different functional forms for the correlation energy and setting parameters for the hopping lead to some difference in results for anisotropic masses. It is obvious that these can cause the difference in the band curvatures and, therefore, effective masses along the armchair and the zigzag directions. The latter motivate us to use in calculations of binding energies of magnetoexcitons and DMCs the different sets of masses from Refs. [1, 82–84] that allows to understand the dependence of the binding energy of magnetoexcitons and DMCs on effective masses of electrons and holes and the role of anisotropic masses. The corresponding reduced masses $\mu_x$ and $\mu_y$ along the armchair and zigzag directions, respectively, are given in Table I. We use these masses as input parameters and refer to them as the set 1, the set 2, the set 3, and the set 4. Below, we report results for the sets of masses 1 and 3 since they give an upper and lower bounds on the binding energies and the energy contribution from the magnetic field to the binding energies of the Rydberg states. Results from the sets of masses 2 and 4 fall within results of the sets 1 and 3.

A numerical solution of the Schrödinger equation (4), using the aforementioned interaction potentials and input parameters from Table I, is performed using the finite element method, which yields pairs of eigenenergies and eigenfunctions which are solutions to the Schrödinger equation, corresponding to the most-strongly-bound states. The method is based on using the finite element method implemented in Wolfram Mathematica in the NDEigensystem function. We modify the code successfully implemented in Ref. [36] in a way that it explicitly contains $\frac{e^2}{4\pi\epsilon}B^2x^2$ and $\frac{e^2}{4\pi\epsilon}B^2y^2$ terms. Our results for the binding energies of direct excitons in FS and encapsulated hBN phosphorene monolayers and indirect excitons in FS phosphorene bilayer for the masses sets 1 and 3 are given in Table II. One can see that the binding energy of excitons in FS and encapsulated monolayers significantly depend on the anisotropic reduced masses. Moreover, a much lower screening of excitons in the freestanding monolayer makes their binding energies, for example, in the ground state over three fold bigger than when the monolayer is encapsulated by hBN.

To check the validity of the code, we use the input parameters from respective papers listed below and calculate the binding energies of direct and indirect excitons. The code reproduces the theoretical binding energies of direct excitons in phosphorene and of indirect excitons in bilayer reported in Ref. [3], where binding energies are calculated using Wannier effective-mass theory in 2D space, within 8%. The binding energies for $1s$ state obtained using a semi-analytical perturbation theory approach [54] are reproduced within 4%. The code reproduces binding energies for $n = 0, ..., 4$ states for FS phosphorene, phosphorene on SiO$_2$ substrate, and encapsulated by hBN phosphorene.
TABLE II. Binding energies of direct magnetoexcitons in FS and encapsulated hBN phosphorene monolayers and indirect magnetoexcitons in FS phosphorene bilayer for the sets of masses 1 and 3. For indirect magnetoexcitons in the bilayer phosphorene binding energies are calculated using $V_{RK}$ and $V_C$ potentials. Energies are given in meV.

| State | Monolayer | Bilayer |
|-------|-----------|---------|
|       | hBN Set 1 | FS Set 3 | hBN Set 1 | FS Set 3 |
| $1s$  | 187.94    | 718.71  | 199.66    | 746.06    |
| $2s$  | 78.62     | 488.84  | 74.37     | 478.75    |
| $3s$  | 53.83     | 394.04  | 50.35     | 377.72    |
| $4s$  | 35.67     | 319.55  | 32.03     | 311.22    |

when energies obtained using numerical procedure where the Schrödinger equation is solved via a finite element representation of the exciton wave equation [87] within 1% and using $k \cdot p$ theory [88] within 4%.

A. Contribution from the external magnetic field to binding energies of magnetoexcitons in a monolayer

In Fig. 3 (a)-(b) we report the energy contribution from the external magnetic field to the binding energies of Rydberg states for direct magnetoexcitons in FS and encapsulated by hBN phosphorene, respectively, as a function of $B^2$. We report results for the sets of masses 1 and 3. The dashed and solid boundary curves in Fig. 3 correspond to the results obtained with the sets of masses 1 and 3, respectively. The results from the sets of masses 2 and 4 fall in the shaded region.

Interestingly enough, in phosphorene, we observe the same tendencies for magnetoexcitons as in TMDCs [23, 67] and Xenes [27] monolayers. The binding energies and the energy contribution from the magnetic field to the binding energies of Rydberg states of magnetoexcitons strongly depend on the exciton reduced mass, even though phosphorene has anisotropic mass along $x$ and $y$ directions. The reduced mass of the exciton along the AC direction, depending on the set, is between seven and fifteen times smaller than the reduced mass along the ZZ direction. Since according to Eq. (4), the Schrödinger equation contains terms that are proportional to $\frac{1}{\mu_x}$ and $\frac{1}{\mu_y}$, the terms with significantly smaller $\mu_x$ dominate in Eq. (4). This is consistent with the anisotropic behavior of the potential $W(x, y)$ shown in Fig. 2 that exhibits the anisotropy with respect to the armchair and zigzag directions. Since the set 1 has the lowest $\mu_x$ and the highest $\mu_y$, the set 3 is vice versa, we report results for the sets 1 and 3 as representative cases.

FIG. 3. Dependencies of the energy contribution from the magnetic field to the binding energies of magnetoexcitons in states $1s$, $2s$, $3s$, and $4s$ for FS (a) and encapsulated by hBN (b) phosphorene monolayers on the squared magnetic field. The boundary dashed and solid curves correspond to the sets of masses 1 and set 3, respectively. The contributions for the sets of masses 2 and 4 fall within the shaded region. The inset in Fig. 3 (b) shows the dependence of the energy contribution from the magnetic field on the ratio $\frac{\mu_y}{\mu_x}$.
Here should be noted that in contrast to binding energies of direct excitons in TMDCs and Xenes, the binding energies of direct excitons in phosphorene have more complicated dependence on the anisotropic reduced masses. In phosphorene the central symmetry is strongly broken due to the large anisotropy of the electron and hole effective masses. This can be observed, for example, in the encapsulated by hBN phosphorene. The insert in Fig. 3(b) shows the dependence of the magnetic field contribution to the binding energy of the direct magnetoexciton on the ratio $\mu_y/\mu_x$. Here we plot $\Delta E$ using the values $\mu_x$ from Table I for $\mu_y = 8, 9, 10, 11, 12.5$ and 14 are calculated by extrapolation of $\mu_x$ from Refs. [1, 82–84] and obtaining corresponding $\mu_y$ using the value of $\mu_x$. The bigger $\mu_y/\mu_x$ ratio corresponds to the more anisotropic system that becomes quasi-one-dimensional [82], and the increase of $\mu_y/\mu_x$ leads to the increase of the contribution due to the magnetic field to the binding energy of the magnetoexciton. The character of these magnetoexcitons is that their spatial distribution of wave functions is strongly anisotropic. These magnetoexcitons form striped-like patterns, similar to those in nanotubes [89] or nanowires [90] that are 1D systems.

Interestingly, the set 1 with the lowest $\mu_x$ and the highest $\mu_y$ has the lowest 1s state binding energy, but for states 2s, 3s, and 4s the set 3 with the highest $\mu_x$ and the lowest $\mu_y$ gives the lowest binding energies. The binding energy percent difference between the sets 1 and 3 in states 2s, 3s, and 4s is 6%, 7%, and 11%, respectively. Also, based on Fig. 3(a), for states 1s-3s the set 1 gives the highest energy contribution to the binding energy and the set 3 gives the lowest $\Delta E$. However, for the state 4s the trend is reversed, and the set 3 gives the highest $\Delta E$, and the set 1 gives the lowest $\Delta E$. In addition, in contrast to magnetoexcitons that dissociate in the TMDCs and Xenes monolayers encapsulated by hBN [27], in states 3s and 4s the magnetoexcitons in phosphorene monolayers stay bound when the magnetic field is varied in the range from 0 to 60 T. This feature is also the result of quasi-1D character of magnetoexcitons in phosphorene.

B. Contribution from the external magnetic field to the binding energies of magnetoexcitons in bilayer and vdW heterostructure

![Diagram](image)

FIG. 4. The energy contribution from the magnetic field to the binding energy of Rydberg states 1s-4s for the FS bilayer obtained using $V_{RK}$ and $V_C$ potentials. The boundary dashed and solid curves correspond to the sets of masses 1 and 3, respectively. The yellow and green shaded areas correspond to the calculations with $V_{RK}$ and $V_C$ potentials, respectively.
For indirect magnetoexcitons in the FS bilayer phosphorene and the vdW heterostructure, we examine how interaction potential affects Rydberg states binding energies and the energy contribution from the external magnetic field to the binding energies. In addition, for the vdW heterostructure, we consider an additional degree of freedom to tune binding energies by number of hBN layers that separate two phosphorene monolayer.

In Fig. 4, we report results for FS bilayer for the sets 1 and 3. The set 1 gives an upper bound on the energy contribution and is denoted by the dashed line. The set 3 gives a lower bound on $\Delta E$ and is denoted by the solid line. As was observed in the monolayer, in the state 4s in bilayer there is a flip of boundaries: the set 1 gives a lower boundary and the set 3 gives an upper boundary. Similar to results reported for magnetoexcitons in Xenes and TMDCs bilayer systems in Ref. [23, 27], in phosphorene bilayer, the following relation always holds $\Delta E_{\text{RK}} > \Delta E_{\text{C}}$. In addition, it is worth mentioning that energy contribution from the magnetic field to the binding energy is higher for indirect magnetoexcitons in the FS bilayer system than for direct magnetoexcitons in FS phosphorene. Based on the results in Table II for the bilayer phosphorene, Rydberg states binding energies calculated with the Coulomb potential are twice as big as the binding energies calculated with the Rytoval-Keldysh potential. Similar to the monolayer system, magnetoexcitons in the bilayer in states 2s, 3s, and 4s are more bound than magnetoexcitons in TMDCs bilayer system.

For the vdW heterostructure, in Fig. 5 we compare $\Delta E_{\text{RK}}$ and $\Delta E_{\text{C}}$. Results are given for the set 3 that is taken to be the representative case. We plot $\Delta E$ as a function of the external magnetic field and the number of hBN layers. As can be seen from Fig. 5 as the number of hBN layers increases $\Delta E_{\text{RK}}$ and $\Delta E_{\text{C}}$ converge. Once
TABLE III. Binding energies for indirect excitons in the van der Waals heterostructures calculated using \( V_{RK} \) and \( V_C \) potentials for the set of masses 3. Energies are given in meV.

| \( N \) | \( V_{RK} \) | \( V_C \) |
|-------|-------|-------|
|       | 1s    | 2s    | 3s    | 4s    | 1s    | 2s    | 3s    | 4s    |
| 1     | 98.50 | 55.13 | 37.45 | 28.11 | 128.38| 66.00 | 43.02 | 30.91 |
| 2     | 86.39 | 51.29 | 35.27 | 27.15 | 104.90| 58.98 | 43.02 | 30.91 |
| 3     | 76.91 | 47.76 | 33.31 | 26.15 | 89.28 | 53.38 | 36.34 | 27.96 |
| 4     | 69.32 | 44.60 | 31.55 | 25.16 | 78.03 | 48.84 | 33.90 | 26.64 |
| 5     | 60.10 | 41.80 | 29.96 | 24.30 | 69.49 | 45.06 | 31.82 | 25.43 |
| 6     | 57.93 | 39.31 | 28.53 | 23.29 | 62.75 | 41.88 | 30.03 | 24.32 |

again, in contrast to indirect magnetoexcitons in TMDCs and Xenes double-layer heterostructure, magnetoexcitons in the vdW phosphorene heterostructure stay bound in states 3 and 4 while the magnetic field is varied between 0 and 60 T. This can be explained by the fact that the binding energies of states 3 and 4 are higher for indirect magnetoexcitons in phosphorene due to their effectively quasi-one-dimensional nature. The quasi-one-dimensionality of the magnetoexcitons in phosphorene is also demonstrated by the comparison of the contribution of the external magnetic field to binding energies of the vdW phosphorene heterostructure shown in Fig. 5 and TMDC heterostructures: \( \Delta E \) due to the magnetic field in the vdW phosphorene heterostructure is always higher than the one in TMDC heterostructures. We report in Table III the binding energies of Rydberg states 1, 2, 3, and 4 for \( N = 1, 2, 3, 4, 5, 6 \) when Eq. 4 is solved with \( V_{RK} \) and \( V_C \). The binding energies calculated using the Coulomb potential are always larger than the one obtained with the RK potential. The increase of the phosphorene interlayer distance in the vdW heterostructure leads to the deduction of electron-hole interaction and results in the decrease of the binding energy of indirect magnetoexcitons.

IV. DIAMAGNETIC COEFFICIENTS

In this paper, we calculate the diamagnetic coefficients in the same fashion as was done in Refs. \[23, 27, 67\]. For phosphorene the diamagnetic coefficients for magnetoexcitons Rydberg states are reported for the first time. The magnetic field range between 0 and 30 T has been used to calculated the DMCs. In this range of the magnetic field one can observe the linear dependence of energy on \( B^2 \). Here, we follow the notation in literature and denote the diamagnetic coefficient as \( \sigma \). The diamagnetic coefficients for magnetoexcitons in monolayer and bilayer systems are reported in Table IV. \( \sigma \) for the indirect magnetoexcitons in the vdW heterostructure are reported in Table V.

TABLE IV. The diamagnetic coefficients, \( \sigma \), of direct magnetoexcitons in FS and encapsulated by hBN monolayers for the sets of masses 1 and 3. \( \sigma \) is given in \( \mu \text{eV}/B^2 \). DMCs are obtained for the range of the magnetic field between 0 and 30 T and correspond to \( R^2 = 0.9998 \) for the linear regression model.

| State | Monolayer | Bilayer |
|-------|-----------|---------|
|       | Set 1     | Set 3   | Set 1     | Set 3   |
|       | hBN | FS | hBN | FS | \( V_{RK} \) | \( V_C \) | \( V_{RK} \) | \( V_C \) |
| 1s    | 0.94 | 0.41 | 0.46 | 0.21 | 0.97 | 0.44 | 0.52 | 0.23 |
| 2s    | 2.31 | 0.68 | 1.41 | 0.40 | 1.34 | 0.55 | 0.80 | 0.32 |
| 3s    | 4.13 | 0.99 | 2.96 | 0.67 | 1.81 | 0.71 | 1.22 | 0.47 |
| 4s    | 1.34 | 1.88 | 1.88 | 1.88 | 2.32 | 0.93 | 3.30 | 1.30 |

We report the diamagnetic coefficients in Table IV for two sets of masses. \( \sigma \) for the FS and encapsulated by hBN monolayers phosphorene is obtained when the magnetoexcitons interact through the \( V_{RK} \) interaction, while for the bilayer \( \sigma \) is given when Eq. 4 is solved using both \( V_{RK} \) and \( V_C \) potential. In the monolayer \( \sigma_1 > \sigma_3 \), where \( \sigma_1 \) and \( \sigma_3 \) are DMCs obtained with sets of masses 1 and 3, respectively. For phosphorene encapsulated by hBN, \( \sigma \) can be extracted in states 1s, 2s, and 3s. In the case of FS phosphorene \( \sigma \) can also be extracted in the state 4s. In the case of bilayer phosphorene, the diamagnetic coefficients can be extracted for 1s, 2s, 3s, and 4s states. This is different to the diamagnetic coefficients of bilayer composed of Xenes \[27\] and TMDCs \[23\], where \( \sigma \) cannot be extracted for all examined states.
TABLE V. The diamagnetic coefficients, $\sigma$, of indirect magnetoexcitons in the vdW heterostructure for the sets of masses 1 and 3. $\sigma$ is given in $\mu$eV/B$^2$. DMCs are obtained for the range of the magnetic field between 0 and 30 T and correspond to $R^2 = 0.9998$ for the linear regression model.

| State | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
|-------|---------|-------|---------|-------|
|       | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
|       | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
|       | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
|       | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
|       | $V_{RK}$ | $V_C$ | $V_{RK}$ | $V_C$ |
| 1s    | 2.36    | 1.72  | 1.24    | 0.88  |
| 2     | 2.80    | 2.22  | 1.49    | 1.16  |
| 3     | 3.23    | 2.72  | 1.74    | 1.45  |
| 4     | 3.67    | 3.20  | 2.00    | 1.73  |
| 5     | 4.09    | 3.68  | 2.27    | 2.02  |
| 6     | 4.51    | 4.14  | 2.53    | 2.30  |

The DMCs for the vdW heterostructure are reported in Table V for two sets of masses when Eq. (4) is solved using $V_{RK}$ and $V_C$ potentials. $\sigma$ can be extracted for the state $1s$ for all values of examined $N$, in the state $2s$ for the set $3$ $\sigma$ can be extracted for $N = 1, ..., 6$. But for the set 1 in the state $2s$, $\sigma$ can be extracted only for $N = 1, ..., 4$. From data listed in Tables IV and V it follows that $\sigma_{RK} > \sigma_C$, where $\sigma_{RK}$ and $\sigma_C$ are the DMCs obtained using the Rytov and Coulomb potentials, respectively. Finally, our calculations show that the magnetoexcitons binding energies and DMCs in phosphorene vdW heterostructure can all be broadly tuned by changing the number of stacked hBN layers. This serves as a convenient and efficient method for engineering the materials properties.

V. CONCLUSIONS

In the framework of the excitonic Mott-Wannier model, we study direct and indirect excitons in Rydberg states in phosphorene monolayers, bilayer, and vdW heterostructure in the external magnetic field, applied perpendicular to the monolayer or heterostructure. We calculated the binding energies and DMCs for the Rydberg states $1s$, $2s$, $3s$, and $4s$ for magnetoexcitons formed in these systems.

The magnetic field contribution to the binding energy of magnetoexcitons strongly depends on the effective masses of electron and hole and their anisotropy. Interestingly, the binding energies of magnetoexcitons are strongly correlated with the reduced mass anisotropy that makes magnetoexcitons in phosphorene effectively quasi-1D quasiparticles. An overall, the unique anisotropic character of these magnetoexcitons in phosphorene leads to the larger contribution to the binding energy than in TMDC materials.

The DMCs demonstrate the strong dependence on the effective electron-hole masses: DMCs in phosphorene monolayers, bilayer, and vdW heterostructure for the set 1 are about two fold bigger than the one for the set 2. The other distinct feature for the diamagnetic coefficients in the bilayer and vdW heterostructures is that $\sigma$ calculated using the Coulomb potential is always smaller than DMCs obtained with the Rytova-Keldysh potential. In other word, the reduced dimensionality and screening increase the diamagnetic coefficients.

We show that the binding energy of direct and indirect magnetoexcitons can be tuned by the external magnetic field. Also, the binding energy of indirect excitons and DMC could be efficiently tuned by the stacking hBN layers. Such tunability of binding energies and DMCs is potentially useful for the devices design.

Finally, in summary, we have shown theoretically that the vdW phosphorene heterostructure is a novel category of 2D semiconductor offering a tunability of the binding energies of magnetoexcitons by mean of the external magnetic field and control by the number of hBN layers separating two phosphorene sheets. Also, the DMCs in the vdW heterostructure are tunable by controlling the number of hBN layers that separate two phosphorene layers. Thus, phosphorene provides a unique platform for novel optoelectronic applications and the exploration of the role of the symmetry breaking in anisotropic exciton physics.

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