

Magnetoexcitons in phosphorene monolayers, bilayer, and van der Waals double-layer heterostructures

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Abstract

We study direct and indirect excitons in Rydberg states in phosphorene freestanding (FS) and encapsulated by hBN monolayers, FS bilayer, and van der Waals (vdW) double-layer heterostructures, when the external magnetic field is applied perpendicular to the examined systems, within the effective mass approximation framework. By a numerical integration of the Schrödinger equation, we obtain binding energies of magnetoexcitons. The interaction potential between electron and hole in a monolayer is taken to be the Rytova-Keldysh (RK) potential while in bilayer and vdW heterostructures the interactions are described by both the RK and Coulomb potentials. The latter allows to address the role of screening in phosphorene. We report the energy contribution from the magnetic field to the binding energies of Rydberg states and diamagnetic coefficients (DMCs) and their strong dependence on electron and hole masses' anisotropy along x and y directions. We show that the energy contribution and DMCs can be effectively tuned by varying the number of hBN layers that separate two phosphorene monolayers.

Theoretical Model

Phosphorene has a unique topological structure such that electron and hole have asymmetric masses along x (armchair, AC) and y (zigzag, ZZ) directions. Along AC direction electron and hole masses are smaller than along ZZ direction.

The Hamiltonian for electron-hole pair with anisotropic masses in the external magnetic field ($\hbar = c = 1$):

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

where m_i^j , $j = x, y$, $i = e, h$ correspond to the effective mass of the electron or hole in the x or y direction, respectively. $V(|\mathbf{r}_e - \mathbf{r}_h|)$ describes the electrostatic interaction between electron and hole. For direct excitons, the Rytova-Keldysh (RK) potential^{2,3} is used:

$$V_{RK}(\mathbf{r}) = -\frac{\pi k e^2}{2\kappa\rho_0} [H_0(\rho/\rho_0) - Y_0(\rho/\rho_0)] \quad (2)$$

For indirect excitons in bilayer and vdW heterostructure, the RK and Coulomb potentials are used:

$$V_{RK}(\mathbf{r}) = -\frac{\pi k e^2}{2\kappa\rho_0} \left[H_0\left(\frac{\sqrt{\rho^2 + D^2}}{\rho_0}\right) - Y_0\left(\frac{\sqrt{\rho^2 + D^2}}{\rho_0}\right) \right], \quad (3)$$

$$V_C\left(\frac{\sqrt{\rho^2 + D^2}}{\rho_0}\right) = -\frac{k e^2}{\kappa\left(\frac{\sqrt{\rho^2 + D^2}}{\rho_0}\right)} \quad (4)$$

Where $\rho^2 = x^2 + y^2$ and $D = h + Nl_{hBN}$, h and l_{hBN} are phosphorene and hBN monolayers' thicknesses, respectively.

The final Schrödinger equation for relative motion of the electron and hole with zero center-of-mass momentum has the form:

$$\left[-\frac{1}{2\mu_x} \frac{\partial^2}{\partial x^2} - \frac{1}{2\mu_y} \frac{\partial^2}{\partial y^2} + \frac{e^2}{8\mu_x} B^2 x^2 + \frac{e^2}{8\mu_y} B^2 y^2 + V(x, y) \right] \Phi(x, y) = E \Phi(x, y) \quad (5)$$

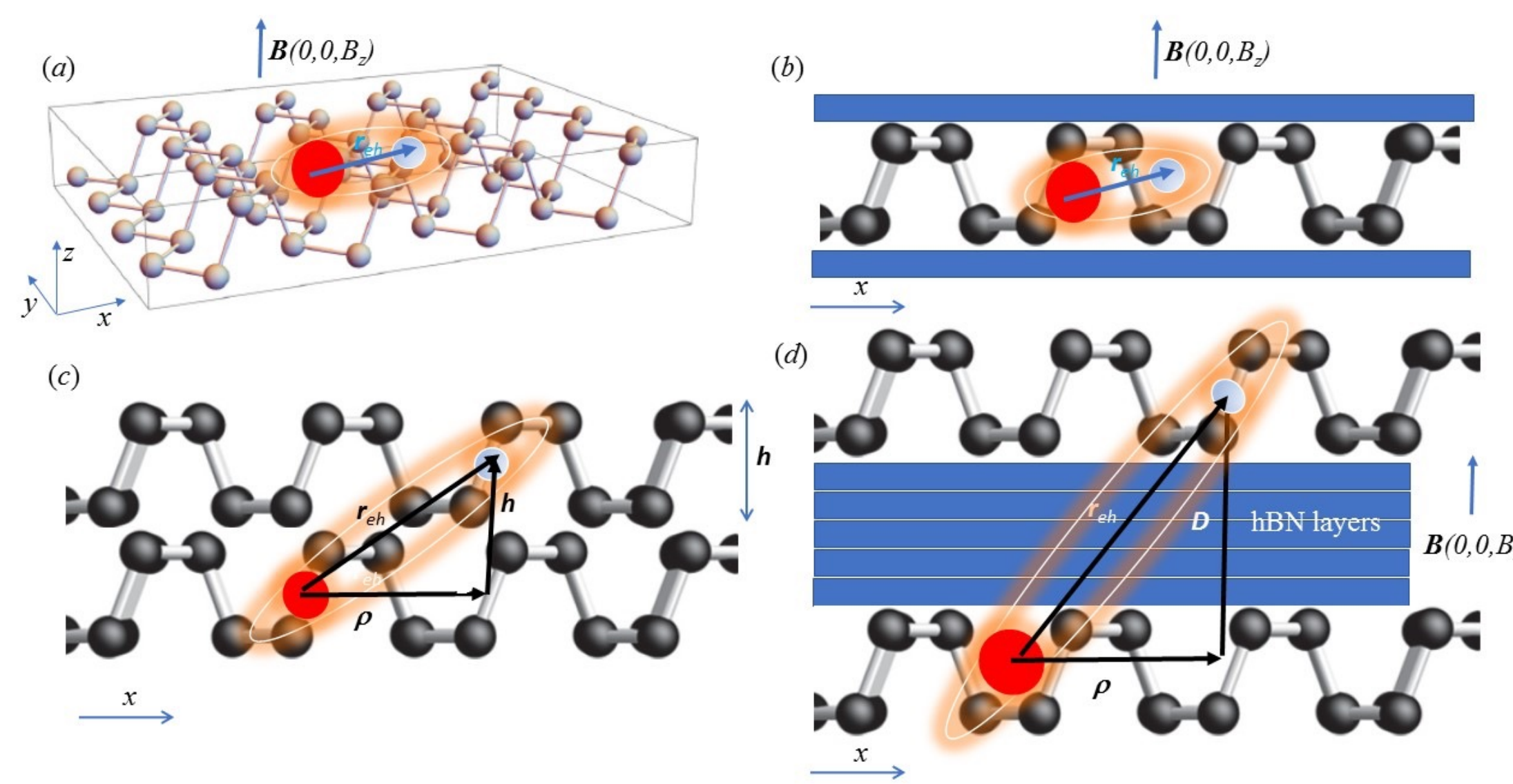


Fig. 1 Schematic illustration of magnetoexcitons in phosphorene monolayers and heterostructures. (a) A direct magnetoexciton in a freestanding phosphorene monolayer. (b) A direct magnetoexciton in an encapsulated phosphorene monolayer. (c) An indirect magnetoexciton in a freestanding bilayer phosphorene heterostructure. (d) An indirect magnetoexciton in phosphorene van der Waals heterostructure.

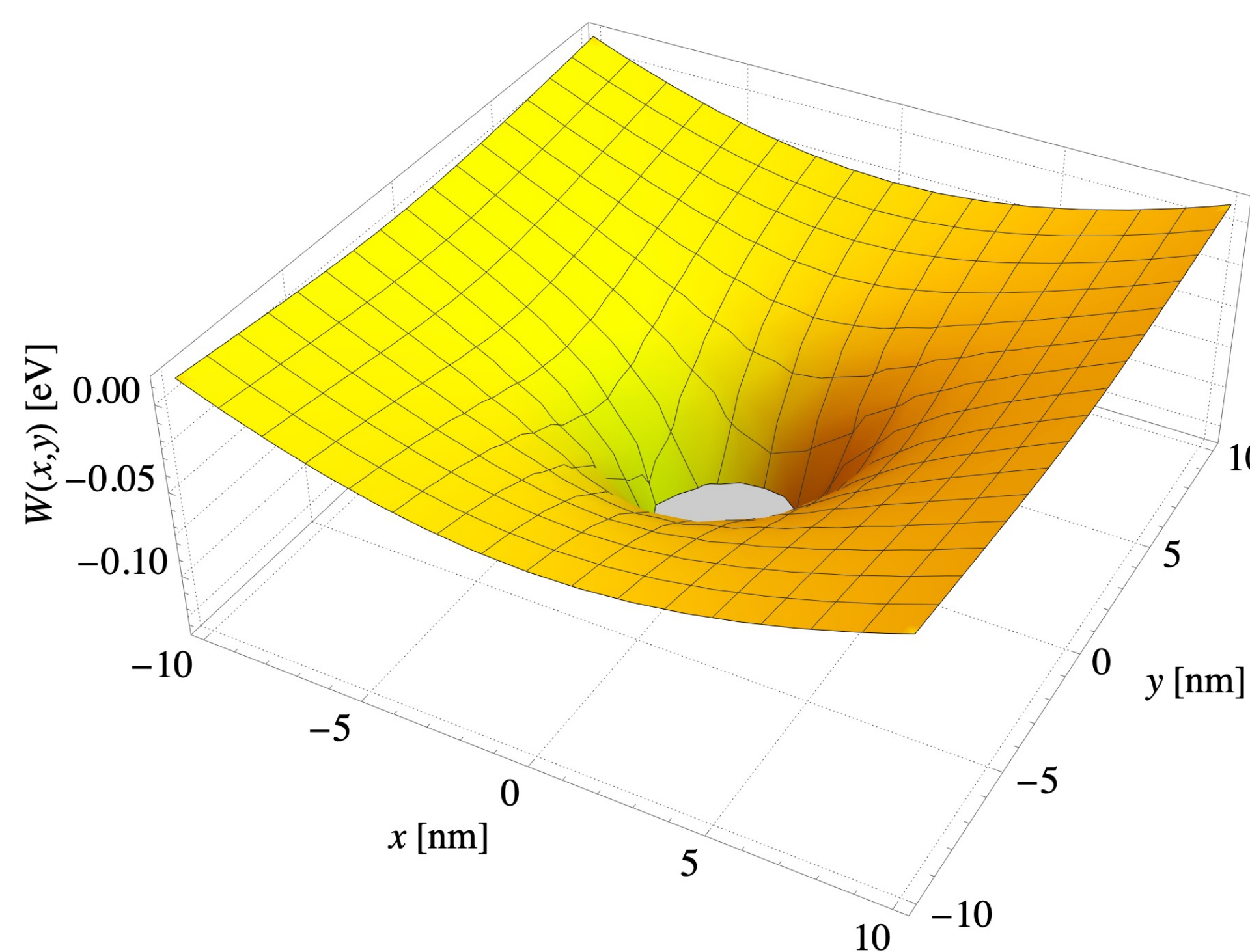


Fig. 2 Total potential

$$W(x, y) = V_{RK} + \frac{e^2}{8\mu_x} B^2 x^2 + \frac{e^2}{8\mu_y} B^2 y^2$$

is plotted as a function of x and y . $W(x, y)$ and x and y are given in eV and nm, respectively. The potential is calculated at $B = 30$ T. The potential demonstrates the anisotropy of phosphorene.

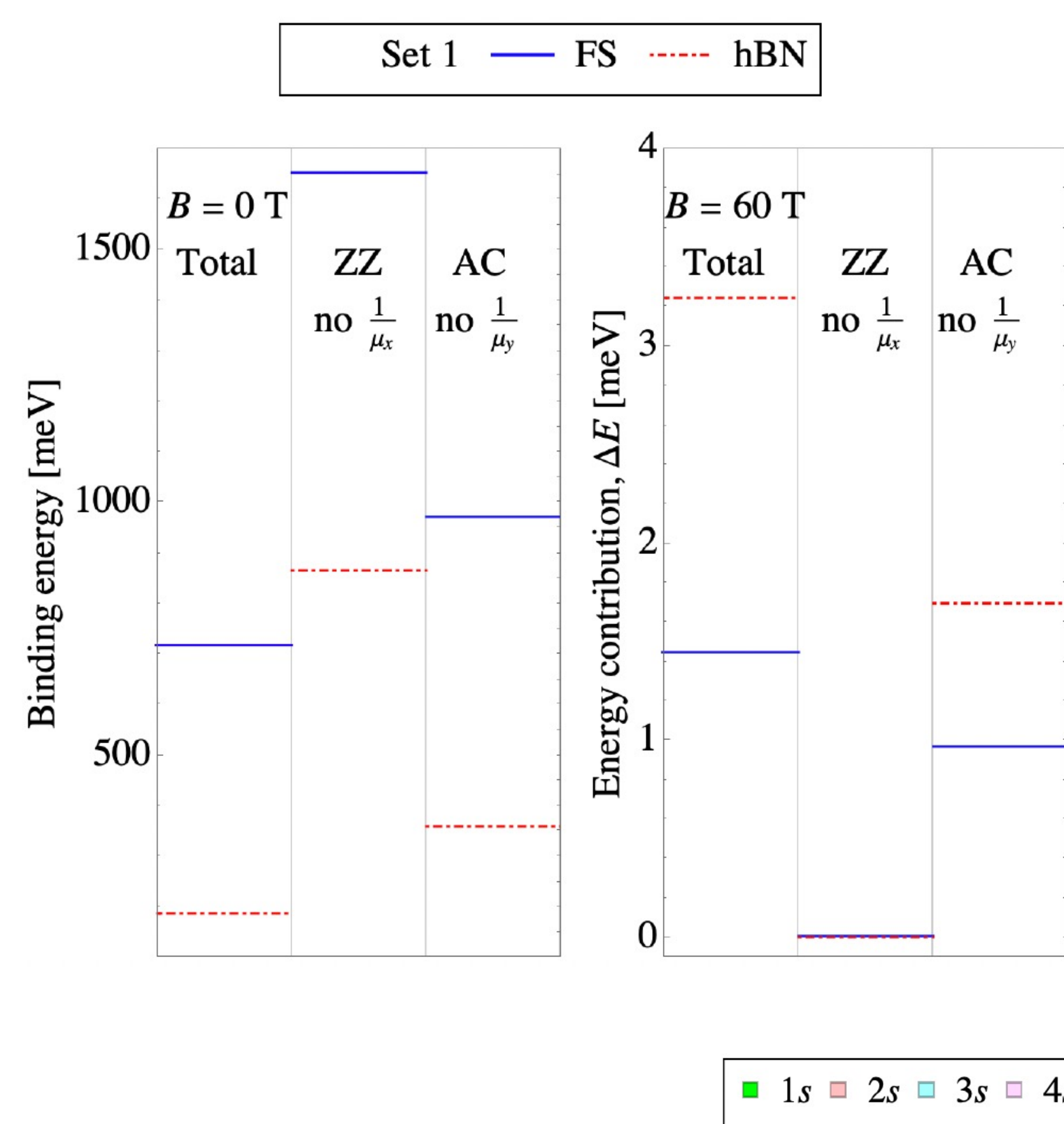


Fig. 3 Diagrams of the energy levels of excitons at $B = 0$ T, and the contribution from magnetic field at $B = 60$ T. Data are given for FS and encapsulated by hBN phosphorene monolayers. The graph shows the binding energy is dominated by $1/\mu_y$ term, while ΔE is dominated by $1/\mu_x$ term.

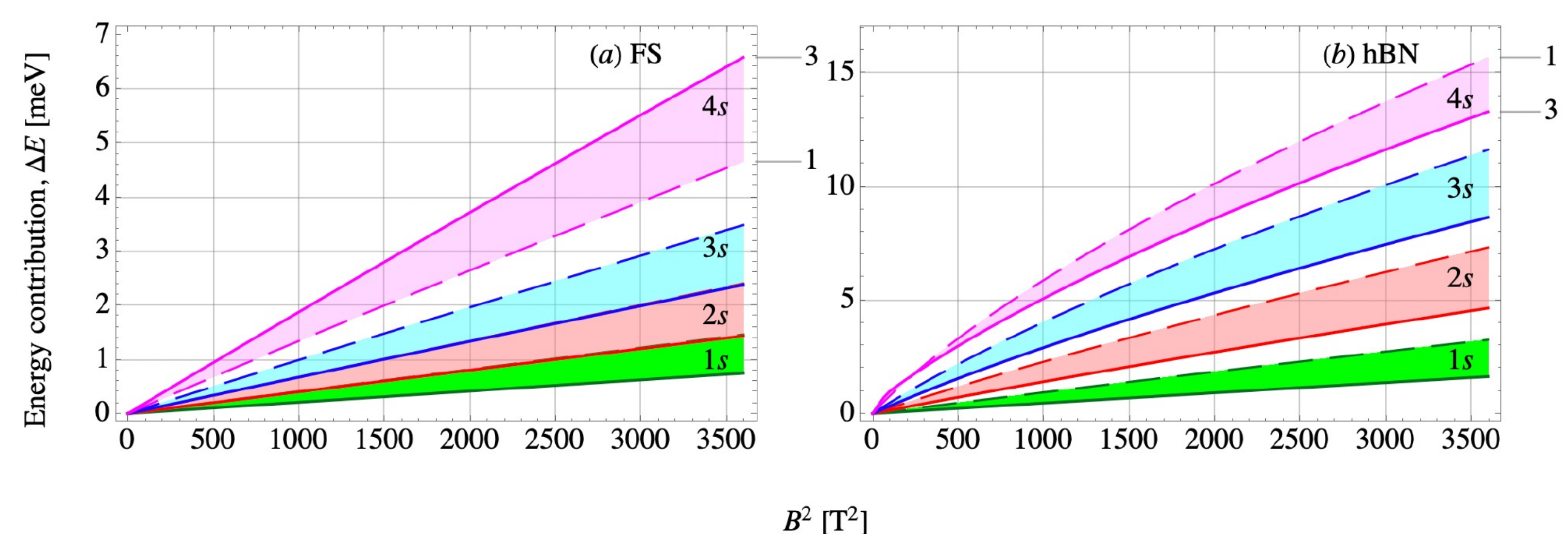


Fig. 4 Dependencies of the energy contribution from the magnetic field to the binding energies of magnetoexcitons in states 1s, 2s, 3s, and 4s for FS (a) and encapsulated by hBN (b) phosphorene monolayers on the squared magnetic field. The boundary dashed and solid curves correspond to the sets of masses 1 and set 3, respectively. The contributions for the sets of masses 2 and 4 fall within the shaded region. The flip of upper and lower bound in state 4s is not an artifact, but the result of the input mass parameters.