# Chapter 129
# Trions in Three-, Two- and One-Dimensional Materials


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**Abstract** The effect of reduction of dimensionality on the Coulomb potential and the binding energy of positively $X^+$ and negatively $X^-$ charged trion is presented. In bulk semiconductors $X^+$ is unbound, while in 2D layered and 1D semiconductors both trions are bound and binding energies of $X^+$ are bigger than $X^-$.

## 129.1 Introduction

The study of a few-body electron-hole system in three-, two- and one-dimensional (3D, 2D, 1D) configuration spaces is of great fundamental significance in physics. Atomic or molecular thin 2D layers and 1D system such as quantum wires and nanotubes allow to address the role of Coulomb interactions in confined geometries. It was realized that for 2D semiconductors, the dielectric environment plays a crucial role and influences the effective strength of the Coulomb potential inside a semiconductor layer [1], which allows the formation of tightly bound two-, three- and four-body electron-hole complexes such as excitons, trions and biexcitons. Excitons and charged trions have been discovered in 2D transition metal dichalcogenides (TMDCs) monolayers. The strong exciton and trion binding in TMDC materials arises from the reduced screening in the 2D geometry as well as effective masses of both the electron and the hole. In fact, screening effects play a fundamental role in determining the electron dynamics and the binding energy of excitonic complexes. Moreover, the screening dictates the optical and transport properties of 2D devices [2].

Although the exciton complexes like trions in solid state physics are very similar to the three-body bound systems in atomic and nuclear physics, there are major differences: i. Screening effects, resulting from the host lattice, make the Coulomb

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force much weaker than in atomic systems; ii. Band effects, which make the effective masses of the electrons and holes smaller than the bare electron mass.

In this short note we address how the reduction of dimensionality affects the binding energy of trions in bulk and low-dimensional semiconductors.

## 129.2 Effects due to the reduction of dimensionality

Wannier-Mott trions in bulk and low-dimensional semiconductors represent a three-body system with two identical particle: $AAB$. Negative $X^-$ and positive $X^+$ trions are formed in semiconductors when an exciton is correlated with an additional electron in a conduction band or hole in a valence band, respectively, and produces complexes with two identical particles: *eeh* or *ehh*. The Schrödinger picture within the framework of the effective-mass potential model approach is well suited to describe Wannier-Mott trions and quantum-confined structures. The corresponding Schrödinger equation for the trion in 3D, 2D and 1D configuration space reads as

$$\left({}^{jD}T + \sum_{i<k}^{jD} V(r_{ik})\right)\Psi_{jD}(r_{12}, r_{23}, r_{13}) = E_{jD}\Psi_{jD}(r_{12}, r_{23}, r_{13}), \qquad (129.1)$$

where index $j = 3, 2, 1$ presents the dimensionality of the space and the position vectors $\boldsymbol{r}_i$ are defined in the $j$D space. In (129.1) ${}^{jD}T = -\frac{\hbar^2}{2m_A}{}^{JD}_{A1}\Delta - \frac{\hbar^2}{2m_A}{}^{JD}_{A2}\Delta - \frac{\hbar^2}{2m_B}{}^{JD}_{B}\Delta$ is a three-body kinetic energy operator, where ${}^{JD}\Delta$ is the Laplace operator for each particle and ${}^{jD}V(r_{ik})$ is a pairwise potential in the $j$D configuration space. One can obtain the expectation value for the ground state energy as $E_{jD} = \left\langle {}^{jD}T\right\rangle + \left\langle \sum_{i<k}^{jD} V(r_{ik})\right\rangle$. The later expression could be viewed as the sum of the average value of the operators of kinetic and potential energies in 3D, 2D and 1D configuration space, respectively, obtained by using the corresponding eigenfunction of the trion $\Psi_{jD}\left(r_{12}, r_{23,}r_{13}\right)$ in 3D, 2D and 1D configuration spaces. The decrease of dimensionality produces a variation in the energy spectrum of the system, as well as affects the Coulomb interaction between an electron and hole. For example, let us consider the effect of the reduction of the dimensionality on the kinetic energy. In the two-body problem when the interaction is described by the Coulomb potential due to the reduction of dimensionality only for the kinetic energy, one can observe that the spectrum of energy is changes from $E_{3D} \sim n^{-2}$ (Rydberg series) in the 3D case, to $E_{2D} \sim (n - 1/2)^{-2}$ in the 2D case. Therefore, for example, the ground state energy increases by a factor of 4. Thus, the reduction of dimensionality decreases the kinetic energy of the 2D exciton due to the decrease of the degrees of freedom from three to two. However, the reduction of dimensionality affects the potential energy of the charged carriers' interaction, while this interaction is still electromagnetic. In

particular, the Coulomb potential due to the decrease of dimensionality is modified to the potential [3] in a 2D system and cusp-type potential in a 1D system:

$$^{3D}V(r) = \frac{ke^2}{\varepsilon r} \Rightarrow ^{2D}V(r) = \frac{\pi ke^2}{(\varepsilon_1+\varepsilon_2)\rho_0}\left[H_0\left(\frac{r}{\rho_0}\right) + Y_0\left(\frac{r}{\rho_0}\right)\right] \Rightarrow ^{1D}V(z) = \frac{\pi ke^2}{\varepsilon(a)}\frac{A}{z-z_0}. \tag{129.2}$$

In (129.2) $k = 9 \times 10^9\,\mathrm{Nm^2/C^2}$, $\rho_0$ is the screening length, $\varepsilon$, $\varepsilon_1$ and $\varepsilon_2$ are the dielectric constants of a bulk and two materials that the 2D layer is surrounded by, respectively, and $H_0(r/\rho_0)$ and $Y_0(r/\rho_0)$ are the Struve function and Bessel function of the second kind, respectively. For $r \gg \rho_0$ the potential has the 3D bare Coulomb tail and becomes $^{3D}V(r)$, while when $r \ll \rho_0$ it becomes a logarithmic potential: $\left(ke^2/\varepsilon\rho_0\right)\left[\ln(r/2\rho_0) + \gamma\right]$, where $\gamma$ is the Euler constant. Thus at $r \ll \rho_0$ the effect of the induced polarization becomes dominant—the $1/r$ singularity is replaced by a weaker logarithmic dependence. For a 1D case in (129.2) a dielectric constant depends on a radius $a$ of a nanowire.

To better understand the difference between the screening in 3D and 2D materials let us follow [2] and consider the effect of the macroscopic polarization induced by a point charge surrounded by a 3D and 2D dielectric medium, respectively. The electric field at a distance $r$ from the charge is the sum of the external field produced by the charge, $e/r^2$, and the induced field due to the polarization of the medium. This charge distribution produces a field of the same functional form $ke/\varepsilon r^2$ and the screening is given by a simple multiplicative renormalization by the dielectric constant $\varepsilon$. In contrast to the 3D case, in the 2D case the system is polarizable only on the plane and induced field is equivalent to the electric field produced by a uniform charge distribution on a circle of radius $r$. As a consequence it will be a function of $r$, but with a functional form substantially different from the electric field $ke/\varepsilon r^2$ and with a nonlocal macroscopic screening showing a logarithmic divergence for small distances [3]. Contrary to the 3D system, where the macroscopic screening is mapped in a dielectric constant, in 2D system the screening is nonlocal so that in the 2D Fourier space it is described by a $q$-dependent macroscopic dielectric function [2, 3], which should be contrasted to the multiplicative renormalization of the charge in 3D case, as seen in (129.2).

There are different models of the effective interaction potential in 1D quantum wire: (i) the singularity of the Coulomb potential is cut off at $r = a$, where $a$ is the radius of a wire, and the effective potential is $^{1D}V(z) \sim (z^2 + a^2)^{-1/2}$; (ii) The effective 1D interaction is modeled as cusp-type Coulomb potential $^{1D}V(z) \sim A(z + r_0)^{-1}$, where the parameters $A$ and $r_0$ are determined self-consistently by employing the eigenfunctions of the lateral confinement of electrons and holes. Figure 129.1 depicts the electric field lines between the interacting electron and hole. For 2D materials field lines are screened in plane and mainly lie unscreened in the vacuum. In 1D materials field lines lie mainly in the vacuum, hence screening is heavily suppressed.

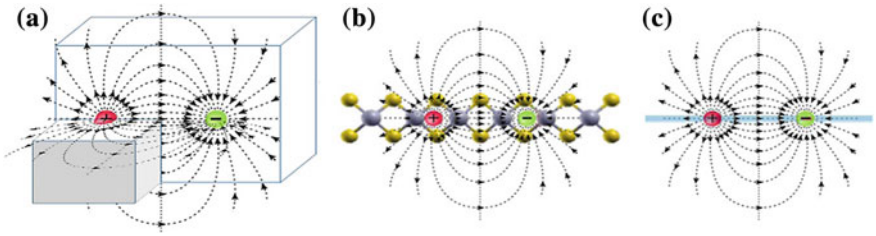


**Fig. 129.1** The scheme of electric fields for two interacting particles in a uniform dielectric environment in 3D, 2D and 1D materials

## 129.3 Binding energy of trions

**3D trions**. Calculations of the binding energies of trions in different 3D materials using the Faddeev equations in configuration space [4] give the following results for $X^-$: 3.6 meV (InN), 0.5 mev (GaAs), 2.1 meV (ZnSe) and 0.6 meV (CdTe) and $X^+$ is unbound. In calculations the ratio of mass $m_e/m_h$ for these materials is varied from 0.07 to 0.27 and for these ratios the exciton binding energies are in good agreement with experimental data and theoretical calculations. The binding energy for $X^-$ and $X^+$ are equal if $m_e = m_h$ or if one ignores the interaction between two identical particles.

In [4] we considered the hypothetical model, which controls the strength of interaction between identical particles for both trions and leads to a weaker Coulomb interaction between the identical particles and hence an increased trion binding energy. Our calculations for the distributions of electrons and holes in $X^{\pm}$ based on the Faddeev equations shows that the $X^-$ has a more extended distribution for two electrons, while the two holes in $X^+$ are considerably closer to each other. Therefore, comparing the interactions of three particles in $X^{\pm}$, one concludes that while the *eh* attraction is the same, the *hh* repulsion is stronger in $X^+$ than the *ee* one in $X^-$ due to more close localization of the two holes. This repulsion reduces the energy of trions so that $X^+$ becomes unbound for all considered dielectric constants.

**2D trions**. Follow [5, 6] for the nonrelativistic trion (129.1) in a 2D configuration space can be written using the formalism of hyperspherical harmonics. Within this approach the binding energies of trions in the TMDCs monolayers are calculated and presented in Table 129.1. Analyses of the results shows that in contrast to 3D

**Table 129.1** The ratio of binding energies $B_{X^+}$ and $B_{X^-}$ of charged trions for different TMDCs that have different ratio of effective electron $m_e$ and hole $m_h$ masses

| | $MoS_2$ | $MoSe_2$ | $MoTe_2$ | $WS_2$ | $WSe_2$ | $WTe_2$ |
|---|---|---|---|---|---|---|
| $m_e/m_h$ | 0.819 | 0.863 | 0.821 | 0.739 | 0.756 | 0.602 |
| $\rho_0$, Å | 38.62 | 51.71 | 73.61 | 37.89 | 34.72 | 49.56 |
| $B_{X^+}/B_{X^-}$ | 1.012 | 1.044 | 1.023 | 1.005 | 1.006 | 1.022 |

case $X^+$ is bound, moreover the binding energy of $X^+$ always exceeds the binding energy of $X^-$.

**1D trions**. The study of $X^\pm$ trions in 1D semiconductor wires within a variational approach [7] and of $X^+$ in the Born-Oppenheimer approximation [8] shows that trion binding energies are defined by two parameters: the mass ratio, $m_e/m_h$, and the radius of the quantum wire $a$. Both $X^+$ and $X^-$ are bound. With the increase of mass ratio $m_e/m_h$ and $a$ the binding energies of $X^\pm$ trions are decreasing, but the $B_{X^+} > B_{X^-}$ and the binding energy $B_{X^+}$ varies more dramatically than $B_{X^-}$.

To conclude, a decrease of dimensionality leads to a decrease of the degrees of freedom in the system, which, obviously, decreases the kinetic energy of the system. At the same time, a decrease of dimensionality reduces the screening that leads to weaker interaction. The combinations of these two effects finally leads to 2D and 1D bound trions because with the reduction of dimensionality the kinetic energy decreases faster than the potential energy, while in 3D $X^-$ is bound and $X^+$ is unbound. Therefore, lowering the dimensionality of the system makes the effects of interaction between particles much more pronounced, resulting in an increase in the binding energy of trions.

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## References

1. Wang, G., Chernikov, A., Glazov, M.M., et al.: Rev. Mod. Phys. **90**, 21001 (2018)
2. Cudazzo, P., Tokatly, I.V., Rubio, A.: Phys. Rev. B **84**, 085406 (2011)
3. Keldysh, L.V.: JETP Lett. **29**, 658 (1979)
4. Filikhin, I., Kezerashvili, R. Ya., Vlahovic, B.: Phys. Lett. A **382**, 787 (2018)
5. Kezerashvili, R. Ya., Tsiklauri, Sh. M.: Few-Body Syst. **58**, 18 (2017)
6. Filikhin, I., Kezerashvili, R. Ya., Tsiklauri, Sh. M., Vlahovic, B.: Nanotechnology **29**, 124002 (2018)
7. Semina, M.A., Sergeev, R.A., Suris, R.A.: Semiconductors **42**, 1427 (2008)
8. Kezerashvili, R. Ya., Machavariani, Z. S., Beradze, B., Tchelidze, T.: Physica E **109**, 228 (2019)