Trions in bulk and monolayer materials: Faddeev equations and hyperspherical harmonics

IOP Publishing Nanotechnology
Nanotechnology 29 (2018) 124002 (7pp) https://doi.org/10.1088/1361-6528/aaa94d

Trions in bulk and monolayer materials: Faddeev equations and hyperspherical harmonics

I Filikhin[1], R Ya Kezerashvili[2], Sh M Tsiklauri[3] and B Vlahovic[1]

[1] Mathematics and Physics Department, North Carolina Central University, Durham, NC 27707, United States of America
[2] Physics Department, New York City College of Technology, The City University of New York, Brooklyn, NY 11201, United States of America
[3] Borough of Manhattan Community College, The City University of New York, USA New York, NY 10016, United States of America

E-mail: RKezerashvili@citytech.cuny.edu

Received 1 October 2017, revised 27 December 2017
Accepted for publication 19 January 2018
Published 9 February 2018

Abstract

The negatively T^- and positively T^+ charged trions in bulk and monolayer semiconductors are studied in the effective mass approximation within the framework of a potential model. The binding energies of trions in various semiconductors are calculated by employing the Faddeev equation with the Coulomb potential in 3D configuration space. Results of calculations of the binding energies for T^- are consistent with previous computational studies, while the T^+ is unbound for all considered cases. The binding energies of trions in monolayer semiconductors are calculated using the method of hyperspherical harmonics by employing the Keldysh potential. It is shown that 2D T^- and T^+ trions are bound and the binding energy of the positive trion is always greater than for the negative trion due to the heavier effective mass of holes. Our calculations demonstrate that screening effects play an important role in the formation of bound states of trions in 2D semiconductors.

Keywords: negative trion, positive trion, binding energy, Keldysh potential, screening effects

(Some figures may appear in colour only in the online journal)

1. Introduction

Excitonic effects in semiconductor nanostructures that are determined by the energies of excitonic complexes such as exciton, trions, biexcitons and the electron–hole interaction, play a critical role in optoelectronic devices and have garnered considerable interest in recent years [1, 2]. Charged exciton complexes such as negative (T^-) and positive (T^+) trions are formed when a single exciton is correlated, respectively, with an additional electron in a conduction band or hole in a valence band, as proposed by Lampert [3]. However, the observation of trions in bulk semiconductors has been hampered due to their rather small binding energies and has become a challenging task. The calculation of the trion wave functions and binding energy is a very old subject that gave rise, in the 1960s and 1970s, to many publications with respect to bulk materials (see, for example, the works [4–6] and citations therein), as well as many calculations for 2D materials after the observation of trions in quantum wells (QWs) by Kheng and co-workers in 1993 [7]. These complexes confined in a QW and in the presence of a magnetic or electric field, have been the subject of extensive theoretical [4–6, 8–25] and experimental [27–40] studies. We cited these articles, but the recent literature on the subject is not limited by them. Theoretical calculations performed at the end of the 1980s [8] predicted a considerable (up to tenfold) increase of the trion binding energy in QW heterostructures compared with bulk semiconductors. Early theoretical calculations by means of variational methods have yielded values of the T^- binding energy for bulk and QWs, which are not too far from the experimental observations. Usually, the solution of the trion eigenequations is very challenging and requires

extensive variational calculations [4–6, 8, 13–16]. For example, in [8] the binding energies for the 3D and 2D trions are calculated variationally using a 22-term Hylleraas-type trial wave function. In the meantime, $T^-$and T^+ trions have been the subject of intense theoretical studies in the past two decades (see, e.g. [18, 26] and references therein). There are stochastic variational calculations that have been done and studies undertaken by means of density functional theory, application of the quantum Monte Carlo method, variational quantum Monte Carlo method, or the diffusion Monte Carlo approach [12, 14, 26, 41, 42]. But, most of these calculations are limited to specific material systems. In order to achieve a better agreement with experimental data, sometimes the problem is treated with a considerable number of fitting parameters.

The binding energies of trions are very small in bulk, but they can be substantially enhanced in structures of reduced dimensionality such as 2D QWs and 1D quantum wires. Calculations have shown that the binding energy of trions is strongly enhanced in 2D structures due to the size-confinement effect A confinement of correlated charge carriers and reduced dielectric screening in these materials led to large many-body effects, resulting in bound-state complexes of electrons and holes with very large binding energies.

After the first work done to demonstrate the existence of charged excitons in monolayer MoS_2 [43], trions have been observed in 2D transition metal dichalcogenide (TMDC) semiconductors with binding energies of 15–30 meV. These binding energies are one order larger than for the trions observed in QWs. Until now, several approaches have been proposed for the evaluation of the binding energies of trions in 2D TMDCs. Trion binding energies in TMDCs were calculated using variational wave functions [44], and more recently using the time-dependent density-matrix functional theory, fractional dimensional space approach, stochastic variational method with explicitly correlated Gaussian basis, the method of hyperspherical harmonics, or quantum Monte Carlo methods, such as the diffusion Monte Carlo and path integral Monte Carlo [44–55].

Although the exciton complexes such as trions in solid-state physics are very similar to the few-body bound systems in atomic and nuclear physics, there is a major difference related to band effects, which makes the effective masses of the electrons and holes smaller than the bare electron mass, and screening effects, resulting from the host lattice, which make the Coulomb force much weaker than in atomic systems. The Mott–Wannier trions in 2D and 3D semiconductors can be described by the solution of the three-body Schrödinger equation after modeling the crystal by effective electron and hole masses and a dielectric constant.

Because trions are intrinsically three-particle objects, common calculation methods are not always adequate to describe their behavior and a more rigorous level of theory must be employed. In the presented work, we study the T^- and T^+ trions in bulk semiconductor within the Faddeev equation formalism [56] and 2D trions in TMDC semiconductors within the framework of the method of hyperspherical harmonics [57, 58]. These methods are the most rigorous approaches for the investigation of a three-body system. In the case of trions, one deals with a three-body system *AAB* with two identical particles. We perform ground-state calculations for $T^{\pm}$ Mott–Wannier trions in the effective mass approximation within the framework of a nonrelativistic potential model using the method of Faddeev equations in 3D configuration space [56] and the method of hyperspherical harmonics in 2D configuration space. In our approach, the trion is a three-particle *AAB* system with two identical particles constituent from electrons and heavy holes, with each pair interacting by the Coulomb potential in the 3D case or in the case of TMDC semiconductors by the screened Coulomb force described via the Keldysh potential [59]. Such an approach allows us to understand the origin of the difference of binding energies for the mirror systems of charged trions.

The paper is organized in the following way. In section 2, a brief description is given of the three-body *AAB* system with two identical particles using the Faddeev equations in 3D configuration space and reduction of the Schrödinger equation using the method of hyperspherical harmonics to a coupled system of differential equations that describe 2D trions in TMDC semiconductors. Results of calculations for the binding energies are presented and analyzed in section 3. The conclusions follow in section 4.

2. Formalism

2.1. 3D trion

Let us consider the formation of trions in a very diluted 2D electron gas with the electron concentration $n \ll 1/\pi a_B^2$, where a_B is the radius of the 2D exciton and the charged exciton complex is the energetically lowest excitation [40]. At these low electron densities the screening length of the electrons drastically changes, giving rise to a substantial increase in the electrostatic disorder in the sample [35]. In the limit of a very diluted carrier gas, the binding energy of the trion is given by the ground-state energy difference between the exciton and trion. The deviation from this 'bare' value of a trion binding energy takes place with increasing carrier density [37, 40]. In the case of the formation of trions in a very diluted 3D electron gas, the electron concentration $n \ll 1/\frac{3}{4}\pi a_B^3$, where a_B is the Bohr radius of the exciton. In most of the binding energy calculations an 'isolated' trion was considered, which is unperturbed by interaction with 2D electron gas. However, there are a great number of effects, which are not directly connected to the model of an 'isolated' trion, but can also influence the trion binding energy and must be taken into account in real heterostructures. For example, the complex valence band of semiconductors, electronic screening effects, electron-to-hole mass ratio, quite different structure of QW based on CdTe, GaAs, and ZnSe, or monolayer TMSC semiconductors, that vary from sample to sample [39, 40].

The simplest way of distinguishing these two cases is to consider the common part of the binding energy of the three-body system, which should be universal for all

semiconductors, and the contribution of sample-dependent effects [39]. Below, we theoretically study the binding energy of trions within the rigorous methods developed in three-body physics: the method of Faddeev equations and the method of hyperspherical harmonics. Our model is the following. The trion is treated as a three-body Coulomb system in the case of a 3D trion and three-particle system interacted via the Keldysh potential in the case of a 2D trion in TMDC monolayers. The model has no fitting parameters and the inputs are electron and hole effective masses that are obtained within standard methods used in condensed matter physics. Therefore, only three-body universal properties are the subject of this paper.

The Faddeev equations in configuration space for a trion can be written in the form of a system of second-order differential equations [56], which can be reduced to a simpler form for the case of two identical particles. In this case, the total wave function of the system is decomposed into the sum of the Faddeev components U and W, corresponding to the $(AA)B$ and $(AB)B$ types of rearrangements: $\Psi = U + W - \mathrm{PW}$, where P is the permutation operator for two identical fermions.

To separate the center-of-mass and relative motion of three particles, let us introduce a set of mass-scaled Jacobi coordinates for the partition i as follows:

$$\begin{aligned}
\mathbf{x}_i &= \sqrt{\frac{m_j m_k}{(m_j+m_k)\mu}}\,(\mathbf{r}_j - \mathbf{r}_k),\\
\mathbf{y}_i &= \sqrt{\frac{m_i(m_j+m_k)}{(m_i+m_j+m_k)\mu}}\left(\frac{m_j\mathbf{r}_j + m_k\mathbf{r}_k}{m_j+m_k} - \mathbf{r}_i\right),\\
&\quad i \neq j = 1, 2, 3,\\
\mathbf{R} &= \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2 + m_3\mathbf{r}_3}{M}, \qquad M = m_1 + m_2 + m_3, \qquad (1)
\end{aligned}$$

where $\mathbf{r}_i$ and m_i are a 3D coordinate and an effective mass of the ith particle, respectively, and $\mu = \sqrt{\frac{m_i m_j m_k}{m_i+m_j+m_k}}$ is the three-body effective mass. Here, the subscripts i, j and k are a cyclic permutation of the particle numbers. Therefore, we have three sets of the Jacobi coordinates. After separating the motion of the center-of-mass, one can write the set of Faddeev equations in 3D configuration space for the relative motion of three particles when two of them are identical fermions in the following form [60, 61]:

$$\begin{aligned}
(H_0 + V_{AA} - E)U &= -V_{AA}(W - PW),\\
(H_0 + V_{AB} - E)W &= -V_{AB}(U - PW). \qquad (2)
\end{aligned}$$

In equation (2) the Hamiltonian H_0 is the operator of kinetic energy written in terms of corresponding Jacobi coordinates, E is the ground-state energy of a trion, while V_{AA} and V_{AB} are the potentials of the pairwise interactions between the particles. The pairwise interactions in bulk materials are described by the Coulomb potential with the dielectric constant related to the considered material.

Let us consider the states of T^- and T^+ trions with the total angular momentum $L = 0$, the momentum of pair $l = 0$, and momentum $\lambda = 0$ of the third particle with respect to the center-of-mass of the pair. Within this condition, the pair of electrons (holes) is in a singlet spin state. The corresponding spin function is an asymmetric relative to the permutation operator P, which provides automatically the asymmetry of the trion wave function Ψ: $P\Psi = P(U + W - PW) = -U + PW - \mathrm{W} = -\Psi$.

2.2. 2D trion

The nonrelativisic trion Hamiltonian in a 2D configuration space is given by

$$H = -\frac{\hbar^2}{2}\sum_{i=3}^{3}\frac{1}{m_i}\nabla_i^2 + \sum_{i<j}^{3} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|). \qquad (3)$$

In equation (3) $V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|)$, where $\mathbf{r}_i$ is now the ith particle position in a 2D configuration space, is the Keldysh potential [59], which describes the Coulomb interaction screened by the polarization of the electron orbitals in the 2D lattice. After the transformation (1), where we are now considering $\mathbf{r}_i$ as a 2D coordinate of the ith particle, the Schrödinger equation for the relative motion of the three-body system reads

$$\left[-\frac{\hbar^2}{2\mu}(\nabla_{x_i}^2 + \nabla_{y_i}^2) + \sum_{i<j}^{3} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) - E\right]\Psi(\mathbf{x}_i, \mathbf{x}_j) = 0. \qquad (4)$$

To obtain a solution of the Schrödinger equation (4) for the trion, we employ hyperspherical coordinates in 4D configuration space. Let us introduce in 4D space the hyperradius $\rho = \sqrt{x_i^2 + y_i^2}$ and a set of three angles $\Omega_i \equiv (\alpha_i, \varphi_{x_i}, \varphi_{y_i})$, where φ_{x_i} and φ_{y_i} are the polar angles for the Jacobi vectors $\mathbf{x}_i$ and $\mathbf{y}_j$, respectively, and α_i is an angle defined as $x_i = \rho\cos\alpha_i$, $y_i = \rho\sin\alpha_i$. Using these coordinates, equation (4) can be rewritten as [53, 57]

$$\left[-\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial^2\rho} + \frac{3}{\rho}\frac{\partial}{\partial\rho} - \frac{\widehat{K}^2(\Omega_i)}{\rho^2}\right) + \sum_{i>j}^{3} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) - E\right]\Psi(\rho, \Omega_i) = 0, \qquad (5)$$

where $\widehat{K}^2(\Omega_i)$ is the angular part of the Laplace operator in 4D configuration space and known as the grand angular momentum operator [57, 58].

One can expand the wave function of the trion $\Psi(\rho, \Omega_i)$ in terms of the HH that are the eigenfunctions of the operator $\widehat{K}^2$, $\widehat{K}^2(\Omega_i)\Phi_{K\lambda}(\Omega) = K(K+2)\Phi_{K\lambda}(\Omega)$, that present a complete set of orthonormal basis

$$\Psi(\rho, \Omega_i) = \rho^{-3/2}\sum_{K\lambda} u_{K\lambda}(\rho)\Phi_{K\lambda}(\Omega_i). \qquad (6)$$

In equation (6), $u_{K\lambda}(\rho)$ are the hyperradial functions and $\lambda \equiv \{l_x, l_y, L, M\}$, where L is the total orbital angular momentum of the trion with M as its projection, and $K = 2n + l_x + l_y$, $n \geqslant 0$ is an integer number. By substituting (6) into (5) one gets a set of coupled differential equations for the hyperradial

Table 1. Trion $T^{\pm}$ and neutral exciton X binding energies in meV for different bulk semiconductors. m_0 and ϵ are the free electron mass and dielectric constant, respectively.

Material	m_e/m_0	m_h/m_0	ϵ	X	T^-	T^+
InN	0.11	1.63	7.5 [62]	24.88	3.6	—
GaAs	0.067	0.51	12.9	4.83	0.5	—
ZnSe	0.16	0.75	8.6	24.2	2.1	—
GaN	0.2	0.82	8.9	27.57	2.1	—
CdTe	0.096	0.35	10.16	9.91	0.6	—
MoS_2	0.45	0.45	10.7 [63, 64]	26.7	∼0.1	∼0.1

functions $u_{K\lambda}(\rho)$ [53]:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} - \frac{(K+1)^2 - 1/4}{\rho^2} + \kappa^2\right] u_{K\lambda}(\rho) = \frac{2\mu}{\hbar^2}\sum_{\kappa'\lambda'} \mathcal{W}_{K\lambda K'\lambda'}(\rho) u_{K'\lambda'}(\rho), \quad (7)$$

where $\kappa^2 = 2\mu B_T/\hbar^2$, B_T is the binding energy of a 2D trion and the coupling effective potential energy is

$$\mathcal{W}_{K\lambda K'\lambda'}(\rho) = \int \Phi^*_{K\lambda}(\Omega_i) \sum_{i<j}^{3} V_{ij}(|\mathbf{r}_i - \mathbf{r}_j|) \Phi_{K'\lambda'}(\Omega_i) \mathrm{d}\Omega_i, \quad (8)$$

which is defined by averaging of the Keldysh potential using the fully antisymmetrized, with respect to two electrons or two holes for T^- and T^+ correspondingly, hyperspherical functions $\Phi_{K'\lambda'}(\Omega_i)$ [53, 61].

3. Results and discussion

We begin by investigating the 3D or bulk case. The results of our calculations for the binding energies of excitons X and $T^{\pm}$ trions in various bulk semiconductors are presented in table 1. The binding energies for the 3D trions are calculated using the aforementioned Faddeev formalism. For comparison, we present the results of calculations for the binding energy B_2 of the exciton in the same semiconductor. The binding energy of a trion is defined as the difference of the ground-state energies of an exciton and a trion. As the inputs we use the Coulomb potential, the known masses of electrons and holes obtained for various bulk materials and the corresponding dielectric constant ϵ. The binding energies of excitons in different semiconductors vary from a few meV to about 30 meV. However, for the same bulk semiconductors the negatively charged trions are weakly bound, while the positively charged trions are completely unbound. This result seems strange because the binding energy of trions is composed by the same electron–hole attraction of the two excitonic pairs and repulsion between two identical particles: two electrons (case of T^-) or two holes (case of T^+) that have the same electric charge. The only difference is related to the different masses of the electron and the hole. Within our approach of the treatment of 3D trions the origin of a discrepancy for the binding energies of T^- and T^+ trions could only arise for one or more of the following three reasons: (i) the Mott–Wannier model is incorrect or incomplete; (ii) the Mott–Wannier model is in principle correct, but the screening caused predominantly by the valence electrons leads to a weaker Coulomb interaction between the identical particles that reduces trion binding energy and hence requires the modification of the Coulomb potential; iii) the effective masses of electrons and holes used in the model are incorrect.

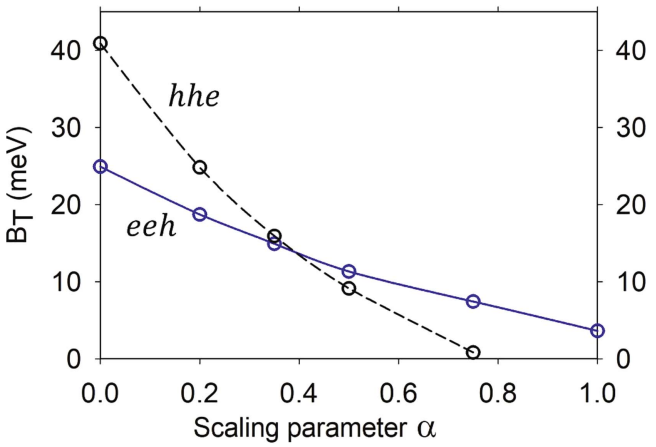

Figure 1. Binding energy B_T for the *eeh* (solid curve) and *hhe* (dashed curve) trions in bulk InN as a function of the scaling factor α for the Coulomb force between identical particles. The calculated values are indicated by open circles.

There is no obvious reason to believe that the Mott–Wannier model, which provides a good description of the Coulomb potential for excitons and a reasonable explanation for the binding energy of the T^- is incorrect. Moreover, this model appropriately provides a good description for excitons and trions in 2D TMDC materials with the Keldysh potential, as shown below. To address the second option, let us introduce the interaction between two identical particles as αV_{AA}, where the parameter α controls the strength of this interaction and varies from 0 to 1. Substituting this potential in equation (2) and solving the Faddeev equations, one can find binding energies B_3 for the T^- and T^+ trions and test the sensitivity of their binding energy to the strength of αV_{AA} by varying the parameter α.

In figure 1, the trion biding energy B_T is presented as a function of the parameter α. The difference between the curves at $\alpha = 0$ shows the contribution due to heavier effective masses of two holes in the *hhe* system relative to the electron masses in the *eeh* system. Thus, the difference of energies of the trions has to depend on the mass ratio. When the interaction between identical particles is omitted ($\alpha = 0$), one can calculate additional energy caused by the mass polarization term of the kinetic operator, known as a mass polarization effect related to the dependence of the binding energy on the mass ratio of non-identical particles of the *AAB* system. The mass polarization energy is different for the *eeh* and *hhe* systems. Therefore, for the trions with different masses of electrons and holes the binding energies of T^+ and T^- have to be different, as one can see in figure 1. The additional analyses show that the slope of the curves is significantly different and the curves intersect at $\alpha = 0.41$. This hypothetical model with parameter α, which controls the

strength of interaction between identical particles, shows that at $\alpha < 0.41$ B_T for the *hhe* system is bigger than for *eeh*, while when $\alpha > 0.41$, we observed the opposite picture: B_T is bigger for the *eeh* and at about $\alpha > 0.78$ $B_T < 0$, which means the *hhe* system is completely unbound. This indicates that the repulsion between identical particles is much stronger in the *hhe* system than in *eeh* because two holes are localized much closer due to their bigger effective masses. Thus, in our hypothetical model with parameter α, which controls the strength of interaction between identical particles for both trions, screening caused predominantly by the valence electrons, leads to a weaker Coulomb repulsion between the identical particles and hence increases trion binding energy. However, this interaction is stronger for two holes because they localized closer to each other than electrons, due the bigger kinetic energy caused by the heavier effective mass of holes, and hence a reduced trion binding energy. Therefore, the effect of the strong repulsion between identical particles due to the Coulomb interaction takes place.

Let us now address the third possibility that the band effective masses of electrons and holes used in the model are incorrect. These masses are taken from *ab initio* calculations, which might not provide a sufficiently accurate description of the electronic band structure. The difference of the electron and hole masses gives appreciable uncertainty in the binding energies for T^-. However, results of our calculations show that the matrix element of the Coulomb repulsion $\langle\Psi|V_{AA}|\Psi\rangle$ between two identical particles cannot be compensated by the mass ratio m_B/m_A effect [65] in the case of T^+. This is related to the fact that hole–hole Coulomb repulsion in T^+ is stronger in considered materials than the electron–electron one in T^- due to the close localization of two holes. Figure 1 illustrates this conclusion. It is obvious that when $\alpha = 0$, the binding energy of the *hhe* system is larger than that of the *eeh* system. We have found that the close localization of the *hh* pair in the *hhe* system is kept for $\alpha = 0.41$, when the binding energies for the *eeh* and *hhe* are equal. The slopes of the curves differ significantly. This indicates that the repulsion between identical particles is much stronger in the *hhe* system than in *eeh* because the two holes are localized much closer to each other due to their larger effective masses.

While bulk, for example, MoS_2 is an indirect gap semiconductor, all 2D TMDC semiconductors becomes direct gap materials with the band gap at the *K*-point of the Brillouin zone. In table 2, we present the summary of the results for the binding energy of T^- and T^+ trions in different TMDC materials obtained by employing the Keldysh potential [59] as input for the *eh*, *ee* and *hh* interactions. In calculations, we use the electron and hole effective masses obtained with the different methods cited in table 2. In particular, we use electron and hole effective masses and r_0 values for the screening length obtained by different *ab initio* methods: many-body G_0W_0 [66] and *GW* [64, 67], density functional theory either in the local density approximation (LDA) [48, 68–73] or using the Perdew–Burke–Ernzerhof (PBE) functional [47, 68, 74–78]. Since a range of masses are reported in the literature, we have taken the average of the reported masses from [55] that were supposedly obtained using the same method. The calculations are performed with the method of hyperspherical harmonics [53, 61]. In all TMDC semiconductors, negatively and positively charged trions are bound. Comparing the binding energies for T^- and T^+ trions one can conclude that T^+ is always stronger bound than T^-. The latter fact has strong correlation with the larger effective mass of the hole than for the electron. Only for one set of the masses for $MoSe_2$ is the energy binding of T^- larger than the one for T^+. However, in this case the effective mass of the electron is bigger than for the hole. The rather small variation in the binding energy of trions in 2D TMDC semiconductors can be well understood from fundamental principles related to their structural and electronic similarities. The small variation of the binding energies for the same TMDC material is related to the different effective masses of the electron and hole, and the screening parameter r_0 obtained within diverse methods. The results are sensitive to the variations of effective masses and in-plane dielectric susceptibility. While the energies for the same TMDC semiconductor depend relatively weakly on the effective masses of electrons and holes, the difference in the binding energies related to the in-plane susceptibility is certainly dominated. When the screening parameter increases, the binding energy decreases for the same TMDC semiconductor as well as for the different TMDC materials. For completeness in our analysis, we should mention that first, the strength of electron screening in 2D TMDC semiconductors presented by the Keldysh potential [59], and second, the confinement of the *eeh* and *hhe* system due to the reduced dimensionality, lead to the existence of the bound state for T^- and T^+ trions.

4. Conclusions

We provide the calculations for the binding energies of trions within the effective mass Mott–Wannier potential model using the most rigorous approaches for description of a few-body system, the Faddeev equations and the method of hyperspherical harmonics in 3D and 2D configuration space, respectively.

The binding energies of the trions are calculated for different bulk materials based on the Faddeev equation for the *AAB* system in 3D configuration space when charges interact via the Coulomb potential. It was found that the binding energy of the negative trion is relatively small, while the positive trion is unbound. We demonstrated that the screening caused, predominantly by the valence electrons, leads to a weaker Coulomb repulsion between the identical particles and can lead to the bound T^+. On the other hand, the reduction of dimensionality from 3D to 2D is a crucial factor for increasing trion stability, and the trion binding energy grows by a factor of 10.

Calculations within the method of hyperspherical harmonics show that in 2D monolayer TMDC semiconductors, due to the reduced dimensionality and strong screening of *eh*, *ee* and *hh*, interactions presented by the Keldysh potential, negatively and positively charged trions are bound and the binding energy of the positive trion is always greater than that

Table 2. Binding energies of T^- and T^+ trions in meV in different TMDC semiconductors. Effective electron m_e and hole m_h masses and the screening distance r_0 used in calculations are taken from the listed references. m_0 is the free electron mass.

	Method	m_e/m_0	m_h/m_0	r_0 (Å)	T^-	T^+
MoS_2	*GW* [64]	0.350	0.428	38.62 [64]	32.80	33.2
	G_0W_0 [66]	0.6	0.54	38.62 [64]	33.6	33.3
	LDA [68–70]	0.495	0.576	36.28 [71]	34.2	34.4
	PBA [47, 68, 74, 75]	0.47	0.575	44.69 [47]	30.3	30.5
$MoSe_2$	*GW* [67]	0.38	0.44	51.71 [44]	27.6	28.8
	G_0W_0 [66]	0.70	0.55	51.71 [44]	31.7	31.3
	LDA [48, 68, 72, 73]	0.59	0.686	39.79 [71]	33.1	33.4
	PBE [47, 68, 74, 76]	0.546	0.643	53.16 [47]	28.4	28.5
$MoTe_2$	G_0W_0 [66]	0.69	0.66	73.61 [47]	21.3	21.2
	LDA [73]	0.64	0.78	73.61 [47]	21.9	22.4
	PBE [76]	0.575	0.702	73.61 [47]	20.4	20.7
WS_2	*GW* [67]	0.27	0.32	37.89 [44]	33.1	33.2
	G_0W_0 [66]	0.44	0.45	37.89 [44]	33.9	33.9
	LDA [48, 68, 72, 73]	0.312	0.422	32.46 [71]	37.4	37.6
	PBE [47, 68, 75, 76]	0.328	0.402	40.17 [47]	32.7	32.9
WSe_2	*GW* [67]	0.29	0.34	45.11 [48]	28.3	28.4
	G_0W_0 [66]	0.53	0.52	45.11 [48]	30.2	30.2
	LDA [48, 68, 72, 73]	0.36	0.476	34.72 [71]	33.9	34.1
	PBE [47, 68, 75]	0.342	0.428	47.57 [47]	27.1	27.2
WTe_2	LDA [68]	0.325	0.46	49.56 [71, 77]	28.3	28.4
	PBE [78]	0.307	0.51	49.56 [71, 75]	27.6	28.2

of the negative trion due to the larger effective mass of the hole. The mass ratios of the election and hole are inverse values for the *eeh* and *hhe* systems. We have shown that the mass polarization effect takes place for the case when the interaction between identical particles is omitted, which results in the additional binding energy for the *eeh* or *hhe* depending on the mass ratio. Thus, the difference of energies of the trions is sensitive to the mass ratio. Our calculations demonstrate that screening effects play an important role in the formation of bound states of trions in 2D semiconductors.

Finally, we can conclude that in the effective mass Mott–Wannier potential model a negatively charged trion in 3D formed via the Coulomb interaction is fragile and the positively charged trion is unbound, but trion complexes in 2D systems formed via the Keldysh potential become stable.

ORCID iDs

R Ya Kezerashvili https://orcid.org/0000-0002-0011-4062

References

[1] Awschalom D D, Bassett L C, Dzurak A S, Hu E L and Petta J R 2013 *Science* **339** 1174
[2] Xiao J, Zhao M, Wang Y and Xiang Zhang X 2017 *Nanophotonics* **6** 1309
[3] Lampert M A 1958 *Phys. Rev. Lett.* **1** 450
[4] Munschy G and Stébé B 1974 *Phys. Stat. Sol.* B **64** 213
[5] Stébé B 1977 *Nuovo Cimento* B **39** 507
[6] Stébé B, Feddi E and Munschy G 1987 *Phys. Rev.* B **35** 4331
[7] Kheng K, Cox R T, Merle dAubigné Y, Bassani F, Saminadayar K and Tatarenko S 1993 *Phys. Rev. Lett.* **71** 1752
[8] Stébé B and Ainane A 1989 *Superlatt. Microstruct.* **5** 545
[9] Wójs A and Hawrylak P 1995 *Phys. Rev.* B **51** 10880
[10] Stébé B, Munschy G, Stauffer L, Dujardin F and J Murat J 1997 *Phys. Rev.* B **56** 12454
[11] Whittaker D M and Shields A J 1997 *Phys. Rev.* B **56** 15185
[12] Usukura J, Suzuki Y and Varga K 1999 *Phys. Rev.* B **59** 5652
[13] Stébé B and Moradi A 2000 *Phys. Rev.* B **61** 2888
[14] Riva C, Peeters F M and Varga K 2000 *Phys. Rev.* **61** 13873
[15] Stébé B, Moradi A and Dujardin F 2000 *Phys. Rev.* B **61** 7231
[16] Szafran B, Stébé B, Adamowski B J and Bednarek S 2000 *J. Phys.: Condens. Matter* **12** 2453
[17] Dzyubenko A B and Sivachenko A B A B 2000 *Phys. Rev. Lett.* **84** 4429
[18] Peeters F M, Riva C and Varga K 2001 *Physica* B **300** 139
[19] Szlufarska I, Wójs A and Quinn J J 2001 *Phys. Rev.* B **63** 085305
[20] Xie W F 2001 *Phys. Stat. Sol.* B **226** 247
[21] Esser A, Zimmermann R and Runge E 2001 *Phys. Stat. Sol.* B **227** 317
[22] Varshni Y P 2001 *Phys. Stat. Sol.* B **227** 621
[23] Dacal L C O and Brum J A 2002 *Phys. Rev.* B **65** 115324
[24] Dacal L C O, R Ferreira R, Bastard G G and Brum J A J A 2002 *Phys. Rev.* B **65** 115325
[25] Szafran B, Chwiej T, Peeters F M, Bednarek S, Adamowski J and Partoens B 2005 *Phys. Rev.* B **71** 205316

[26] Rønnow T F, Pedersen T G, Partoens B and Berthelsen K K 2011 *Phys. Rev.* B **184** 035316
[27] Finkelstein G, Shtrikman H and Bar-Joseph I 1995 *Phys. Rev. Lett.* **74** 976
[28] Shields A J, Pepper M, Ritchie D A, Simmons M Y and Jones G A C 1995 *Phys. Rev.* B **51** 18049
[29] Buhmann H, Mansouri L, Wang J, Beton P H, Mori N, Eaves L, Henini M and Potemski M 1995 *Phys. Rev.* B **51** 7969
[30] Warburton R J, Durr C S, Karrai K, Kotthaus J P, Medeiros-Ribeiro G and P M Petroff P M 1997 *Phys. Rev. Lett.* **79** 5282
[31] Finkelstein G, Umansky V, Bar-Joseph I, Ciulin V, Haacke S, Ganiere J-D and Deveaud B 1998 *Phys. Rev.* B **58** 12637
[32] Ciulin V *et al* 2000 *Phys. Rev.* B **62** R16310
[33] Esser A *et al* 2000 *Phys. Stat. Sol.* A **178** 489
[34] Esser A *et al* 2000 *Phys. Rev.* B **62** 8232
[35] Esser A, Yayon Y and Bar-Joseph I 2002 *Phys. Stat. Sol.* A **234** 266
[36] Vanhoucke T, Hayne M, Henini M and Moshchalkov V V 2002 *Phys. Rev.* B **65** 041307
[37] Astakhov G V *et al* 2002 *Phys. Rev.* B **65** 165335
[38] Bracker A S *et al* 2005 *Phys. Rev.* B **72** 035332
[39] Sergeev R A, Suris R A, Astakhov G V, Ossau W and Yakovlev D R 2005 *Eur. Phys. J.* B **47** 541
[40] Astakhov G V and Ossau W 2007 *Phys. Stat. Sol.* C **4** 3310
[41] Tsuchiya T 2001 *Int. J. Mod. Phys.* B **15** 3985
[42] Filinov A V, Riva C, Peeters F M, Lozovik E Y and Bonitz M 2004 *Phys. Rev.* B **70** 035323
[43] Mak K F *et al* 2013 *Nat. Mater.* **12** 207
[44] Berkelbach T C, Hybertsen M S and Reichman D R 2013 *Phys. Rev.* B **88** 045318
[45] Thilagam A 2014 *J. App. Phys.* **116** 053523
[46] Ramirez-Torres A, Turkowski V and Rahman T S 2014 *Phys. Rev.* B **90** 085419
[47] Kylänpää I and Komsa H-P 2015 *Phys. Rev.* B **92** 205418
[48] Velizhanin K A and Saxena A 2015 *Phys. Rev.* B **92** 195305
[49] Ganchev B, Drummond N, Aleiner I and Fal'ko V 2015 *Phys. Rev. Lett.* **114** 107401
[50] Mayers M Z, Berkelbach T C, Hybertsen M S and Reichman D R 2015 *Phys. Rev.* B **92** 161404
[51] Zhang D K, Kidd D W and Varga K 2016 *Phys. Rev.* B **93** 125423
[52] Spink G G, López Rós P, Drummond N D and Needs R J 2016 *Phys. Rev.* B **94** 041410
[53] Kezerashvili R Y and Tsiklauri S M 2017 *Few-Body Syst.* **58** 18
[54] Szyniszewski M, Mostaani E, Drummond N D and Fal'ko V I 2017 *Phys. Rev.* B **95** 081301(R)
[55] Mostaani E, Szyniszewski M, Price C H, Maezono R, Danovich M, Hunt R J, Drummond N D and Fal'ko V I 2017 *Phys. Rev.* B **96** 075431
[56] Faddeev L D and Merkuriev S P 1993 *Quantum Scattering Theory for Several Particle Systems* (Dordrecht: Kluwer)
[57] Avery J 1989 *Hyperspherical Harmonics: Applications in Quantum Theory* (Dordrecht: Kluwer)
[58] Jibuti R I and Shitikova K V 1993 Method of hyperspherical functions in atomic and nuclear physics *Energoatomizdat, Moscow* 270 in Russian
[59] Keldysh L V 1979 *JETP Lett.* **29** 658
[60] Filikhin I N, Gal A and Suslov V M 2003 *Phys. Rev.* C **68** 024002
[61] Kezerashvili R Y, Tsiklauri S M, Filikhin I, Suslov V M and Vlahovic B 2016 *J. Phys. G: Nucl. Part. Phys.* **43** 065104
[62] Dvorak M, Wei S-H and Wu Z 2013 *Phys. Rev. Lett.* **110** 016402
[63] Molina-Sanchez A and Wirtz L 2011 *Phys. Rev.* B **84** 155413
[64] Cheiwchanchamnangij T and Lambrecht W R L 2012 *Phys. Rev.* B **85** 205302
[65] Filikhin I, Kezerashvili R Y, Suslov V M and Vlahovic B 2017 On mass polarization effect in three-body systems arXiv:1704.03900v3 [nucl-th]
[66] Ramasubramaniam A 2012 *Phys. Rev.* B **86** 115409
[67] Shi H, Pan H, Zhang Y-W and Yakobson B I 2013 *Phys. Rev.* B **87** 155304
[68] Kormányos A, Burkard G, Gmitra M, Fabian J, Zólyomi V, Drummond N D and Fal'ko V 2015 *2D Mater.* **2** 022001
[69] Kadantsev E S and Hawrylak P 2012 *Solid State Commun.* **152** 909
[70] Yu S, Xiong H D, Eshun K, Yuan H and Li Q 2015 *Appl. Surf. Sci.* **325** 27
[71] Kumar A and Ahluwalia P 2012 *Phys.* B **407** 4627
[72] Jin Z, Li X, Mullen J T and Kim K W 2014 *Phys. Rev.* B **90** 045422
[73] Chang J, Register L F and Banerjee S K 2014 *J. Appl. Phys.* **115** 084506
[74] Yun W S, Han S W, Hong S C, Kim I G and Lee J D 2012 *Phys. Rev.* B **85** 033305
[75] Wickramaratne D, Zahid F and Lake R K 2014 *J. Chem. Phys.* **140** 124710
[76] Liu L, Kumar S B, Ouyang Y and Guo J 2011 *IEEE Trans. Electron Devices* **58** 3042
[77] Lu N *et al* 2016 *J. Phys. Chem.* C **120** 8364
[78] Lu H Y, Lu W J, Shao D F, Liu Y, Tan S G and Sun Y P 2015 *Europhys. Lett.* **110** 37004