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Research Paper

Relativistic Modification of the Exciton's Mass in Monolayer TMDCs Materials

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ABSTRACT

The study of the exotic bound states in atomically thin semiconductors with a transition metal atom has attracted a great deal of interest in quantum field theory. The reality of transition metal dichalcogenide monolayer materials has been the subject of intense concern among theoreticians and experimenters in recent years. To obtain transition metal dichalcogenide monolayer materials with specific properties; it is extremely important to develop particular strategies to obtain specific exotic structures. These exotic structures are considered to be in a two-particle/quasiparticle bound state: exciton and biexciton (exciton-exciton), exciton-polariton, polariton-phonon. Quantum field theory, in its widest sense, is a method to control and achieve reasonable goals. Control of such states enables the control of properties and access to a range of quantum properties, otherwise inaccessible. The relativistic mass spectrum and relativistic constituent mass of particles in monolayer transition metal dichalcogenide monolayer materials have been calculated using the relativistic Schrödinger equation with strong Coulomb-type potential between the electron and hole. The ground state of the transition metal dichalcogenide monolayer has been studied. Therefore, the investigation may indicate promising applications in quantum information processing and electronic device technologies based on the semiconductor quantum dots system.

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1. Introduction

Progress of two-dimensional transition metal dichalcogenide monolayer (2D-TMDCM) semiconductor quantum dots (such as MX2: MoS2, HfSe2, and WSe2) allows exotic constructions, including heavy/light exotic systems, to be synthesized [1, 2]. Specifically, a finite number of excitons can be confined in a bounded volume of the order of normal-sized two-dimensional materials. The 2D-TMDCM materials have recently gained attention in theoretical investigations and experimental explorations. Theoretical physicists are interested in the possibility of controlling the properties of excitons in these materials since these two-dimensional materials can be used as new element bases for future forms and the potential applications of 2D-TMDCM materials in energy storage, sensing applications, and conversion, including electronic devices, excitonic solar cells, electro-photo catalysts, super batteries-capacitors. Electron-hole abnormal atom is the simplest model of bounding states to use when studying the essential features of two (or perhaps more) complicated excitons [3, 4]. Recently, the study of excitons in 2D-TMDCM materials has progressed significantly. Among excitons in 2D-TMDCM materials, a heavy exciton is especially interesting because of their interaction times and the masses of their holes in the bound states (electron transportation has been omitted). Many new exotic bound states have been recently discovered following developments in higher energy interactions than bandgap; exotic systems have become the main topic of studies on semiconductor quantum dots (SQDs) materials and semiconductor technology.

Many theoretical works have focused on determining the relativistic mass of predicated exotic-bound states and the effects of relativistic conditions on them. The present article investigates the asymptotic behavior of the correlation functions of charged fields and the analytic method for determining the mass spectrum and binding energy of heavy/light excitons in 2D-TMDCM materials. According to the results, excitons masses (which I identify as masses of hole-electron in a bound state) differ from hole and electron masses in a free state. This work represents a theoretical and analytical effort—the outcome of this effort, however, resulted in such fundamental quantities as the exotic hole-bound states. This outcome led to make several predictions of the excitons in semiconductor quantum dots. Single hole-atoms are studied using a quantum field theory (QFT) and models. I choose to use the strong Coulomb interaction and phenomenological type potentials, as they play significant roles in SQDs physics. The Schrodinger equation solutions for these potentials are known and can be obtained using various methods. This article calculates the bound state energies of exotic heavy/light excitons in the ground and excited states. Various analytical or numerical approximation methods have been developed to compensate for the fact that the relativistic Schrodinger equation for such a system does not produce solutions. In this way, one can demonstrate the oscillator representation method (ORM) [5, 6] when calculating the mass and binding energy of excitons and comparing the results with phenomenological potential. This technique can be used to accurately describe the characteristics of excitons. Thus, it is essential to developing an ORM in SQDs physics, as it describes the bound-state characteristics of exotic particles such as exciton diexciton, Trion exciton, and multi-exciton systems. Mathcad 15.0 M050 and MATLAB R2020b software are used to determine parameters and calculate their values. All computational and mathematical results were produced by the author.

2. Exciton such as atomic states

Exotic atomic states are those that do not qualify as common, well-known states. Some examples are exciton, biexciton, muonic atoms, and kaonic hydrogens. Let’s consider an exciton confined in a spherical quantum dot of radius embedded in SQDs. The exciton system is a few-body state that has been studied within potential nonrelativistic models and the frameworks of different theoretical/experimental models and methods (e.g., the semi-classical model, Frenkel-exciton model, the unitary model operator, microscopic cluster model, 1/N expansion method, and the adiabatic approximation, the variational method in real space and the

effective-mass theory, multi-Gaussian expansion method, X-ray absorption, and photoemission spectroscopy. However, there is also a method for understanding the exciton state as an atomic state based on the perturbative methods in quantum electrodynamics (QED) at the Nano-scale. It is widely believed that the ORM and QFT are viable perturbative and nonperturbative methods for extracting the characteristics and properties of exciton systems with charged hole-electron particles. However, theoretical and computational works are also available on exotic exciton bound states, especially their wave functions and excited states, eigenvalues. Recently, several new exotic states were observed in experimental investigations of higher energy photon-material collisions. These experimental observations were collected by the National Synchrotron Light Source, Brookhaven National Laboratory and the Advanced Photon Source, Argonne National Laboratory, the Center for Excitonics, Solar Energy Laboratory LESO-PB, Scottish Institute for Solar Energy Research, and Energy Frontier Research Center. A higher aspect and new research fields are expected to be given to exciton physics. Examples include research on exotic systems' properties and characteristics of excitonic cells or quantum excitonic transport, which might become possible using new machines with abundant energy. Therefore, theoretical studies promote awareness and interest in experimental interpretations. Following the last experimental data, I study the hole-electron system as an exotic bound state of a hole and an electron [7, 8]. For the binding energy of the hole-electron state of excitons, I suggest using the Gaussian asymptotic behavior of the correlation functions of the corresponding field currents. This method can determine the energy and mass spectrum in the ground and excited states of exotic two-body systems with electrostatic potential [9]. I also obtained a relativistic correction to the constituent mass of the constituent hole and electron. The mass spectrum is determined using the Schrodinger equation with a mass of constituent components hole and electron Figure 1 and Figure 2.

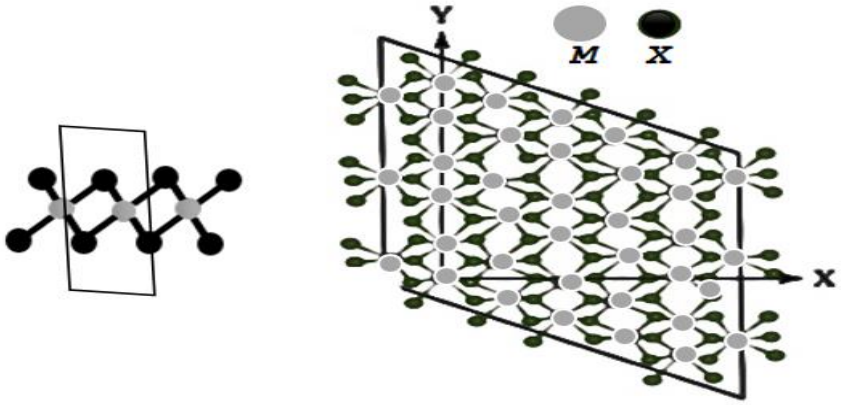

Fig. 1. Side view of the monolayer structures MX_2 in the plane XY.

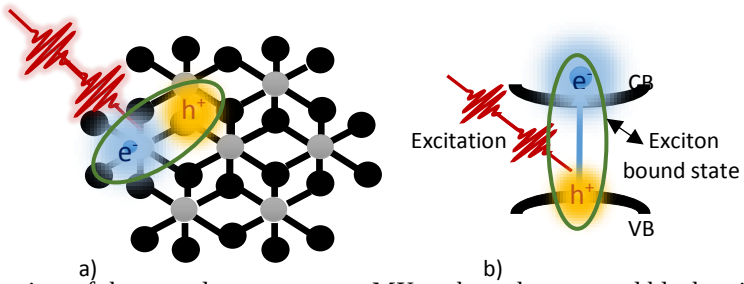

Fig. 2. a) Top view of the monolayer structures MX_2, where the gray and black points represent the M and X elements. b) After the excitation of the MX_2 monolayer, the electron transfers from the valance bands to the conduction bands.

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3. Exciton in TMDCS

Exciton in 2D-TMDCM materials is a quantum system described by strong Coulomb potential with the following range of coupling constants: $\alpha_s \approx 0.09$. I have presented an analytical solution for this system using the Schrödinger equation, which enabled me to determine excitons characteristics and parameters. The Coulomb field becomes present in higher energy interactions among photon-materials, creates a hole that is transferred inside materials, thus forming excitons. Therefore, in this article, the Coulomb potential is used to examine the mass spectra of heavy/light excitons based on ideas and methods related to quantum fields. The Coulomb interaction between these oppositely charged particles results in the formation of a mutual exciton hydrogen atom type bound state [9, 10]; this bound state is called the free exciton and by the Bloch, the theorem is removed by this electron-hole interaction. The exciton moves through the crystal by the diffusion process, just like the individual charged particles. Thus, the mass spectrum and binding energy of excitons were determined through ORM and Feynman path integral techniques [5]. Two-particle m -dimensional Schrödinger equation for exciton in 2D-TMDCM materials (is confined in spherical space with radius R: $R > r_{e.h}$) reads (see Ref. [4] for more details):

$$\left(-\frac{\hbar^2}{2\mu_e^*}\Delta_e - \frac{\hbar^2}{2\mu_h^*}\Delta_h - \frac{e^2}{4\pi\varepsilon_r\varepsilon_0 r} + V_e(r) + V_h(r)\right)\Phi(r) = E(\mu_e^*.\mu_h^*)\Phi(r)$$

$$V_{e.h}(r) = \begin{cases} 0 & \text{if } 0 \le r_{e.h} \le R \\ \infty & \text{if } r_{e.h} > R \end{cases} \quad (1)$$

where μ_e^*, μ_h^* are the effective constituent masses of electrons and holes in the exciton bound state which are different from the effective masses m_e^* and m_h^* (the rest masses of electrons and holes are $m_e = 0.511\text{MeV}, m_h = 0$), r is the electron-hole relative distance concerning the center of the quantum dot, R is the radii of the quantum dot. $V_c(r)$ is the strong Coulomb interaction between the hole and electron, $V_h(r), V_e(r)$ are the potential confinement for a hole, an electron; and for hydrogen-like of bound states such as free exciton: $V_h(r) \approx 0, V_e(r) \approx 0$. ε_r is the dielectric constant of 2D-TMDCM materials. Without loss of generality, the 2D-TMDCM materials SQDs energy bandgap may be set equal to be zero for convenience. ORM is an alternative method of solving total nonrelativistic/relativistic radial Schrödinger equations (for exciton) that are applied for spherically symmetric Coulomb potential and read as follows [4,7]:

$$\left(-\frac{\hbar^2}{2\mu_e^*}\left[\frac{d^2}{dr^2} + \frac{m-1}{r}\frac{d}{dr}\right] - \frac{\hbar^2}{2\mu_h^*}\left[\frac{d^2}{dr^2} + \frac{m-1}{r}\frac{d}{dr}\right] + \frac{\ell(\ell+m-2)}{2\mu^* r^2} + \frac{\ell(\ell+m-2)}{2\mu_h^* r^2} - \frac{e^2}{4\pi\varepsilon_r\varepsilon_0 r}\right)R(r) = E(\mu_e^*.\mu_h^*)R(r) \quad (2)$$

Then

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2} + \frac{m-1}{r}\frac{d}{dr}\right] + \frac{\ell(\ell+m-2)}{2\mu^* r^2} - \frac{e^2}{4\pi\varepsilon_r\varepsilon_0 r}\right)R(r) = E(\mu^*)R(r)$$

$$\frac{1}{\mu^*} = \frac{1}{\mu_e^*} + \frac{1}{\mu_h^*} \quad (3)$$

where $\mu^*$is the reduced effective mass of the two particles, ℓ is the angular quantum number. The application of the ORM implies that a wave function, being a bound ground state of an exciton system with an attractive potential, is expanded over the oscillator basis. In most cases, the asymptotic behavior of a true wave function for short and large distances should coincide with the Gaussian asymptotic behavior of the oscillator wave functions. Therefore, I have to modify the variables in Ref. [1]. Now, based on the asymptotic properties $(r \to \infty, r \to 0)$ of Gaussian type $r = q^{2\rho}$ and $\Psi(r) \to \Psi(r) = q^{2\rho u}\psi(q)$ where $\rho.u$ are parameter to be determined; Using the radial Laplacian operator in the m-dimensional space one can define the radial Laplacian operator in the $\mathcal{D}$-dimensional axillary space [4]:

$$\Delta = \frac{d^2}{dr^2} + \frac{m-1}{r}\frac{d}{dr} \to \Delta_q = \frac{d^2}{dq^2} + \frac{\mathcal{D}-1}{q}\frac{d}{dq}$$

Under this transformation from equation (1) get $(\varepsilon_0 = \hbar = c = 1)$

$$\left(\frac{d^2}{dq^2} + \frac{4\rho u + 2\rho(m-1)+1}{q}\frac{d}{dq} + \frac{4\rho^2\left(u^2 - \ell(\ell+m-2) + u(m-2)\right)}{q^2} + 2\mu^*\rho^2\frac{e^2}{\pi\varepsilon_r q^2}q^{2(2\rho-1)} + 8\mu^*\rho^2 E(\mu^*)q^{2(2\rho-1)}\right)\psi(q) = 0 \quad (4)$$

So that the modified equation should have solutions with the Gaussian asymptotic; in the electrostatic potential, such a modification is performed by $\rho = 1$

where the wave function becomes an oscillator one. Then equation (4) reads as follows:

$$\left(\frac{d^2}{dq^2}+\frac{4u+2m-1}{q}\frac{d}{dq}+\frac{4\left(u^2-\ell(\ell+m-2)+u(m-2)\right)}{q^2}+2\mu^*\frac{e^2}{\pi\varepsilon_r q^2}+8\mu^* E(\mu^*)q^2\right)\psi(q)=0 \quad (5)$$

Then i have to require that Coulomb interaction Hamiltonian does not contain terms quadratic in the canonical variables. This requirement is called the oscillator representation condition in ORM; therefore, the equation (5) with the term q^{-2} set to zero: $\left(u^2-\ell(\ell+m-2)+u(m-2)\right)=0$ and in the particular case $\rho=1$, I determine $s=\ell$. Hence, equation (5) is written in the following form (see Ref. [7] for more details):

$$\left(\frac{d^2}{dq^2}+\frac{4\ell+2m-1}{q}\frac{d}{dq}+2\mu^*\frac{e^2}{\pi\varepsilon_r}+8\mu^* E(\mu^*)q^2\right)\psi(q)=0 \quad (6)$$

$\Omega=\sqrt{-8\mu^* E(\mu^*)}$ is the pure oscillator frequency of exciton system and $\mathcal{D}$-dimensional axillary space determines as follows: $\Delta_q=\frac{d^2}{dq^2}+\frac{\mathcal{D}-1}{q}\frac{d}{dq}\Rightarrow\mathcal{D}=4\ell+2m+2$. Then based on the ORM condition (see Ref. [5] for more details) the canonical variables $\hat{q}^2=\frac{\mathcal{D}}{2\omega}$ and $\hat{p}^2=\frac{\mathcal{D}\omega}{2}$ are obtained through Wick ordering: $\hat{q}=\frac{\hat{a}^-+\hat{a}^+}{\sqrt{2\omega}}$ and $\hat{p}=\sqrt{\frac{\omega}{2}}\frac{\hat{a}^--\hat{a}^+}{2i}$, where $\hat{a}^+$ and $\hat{a}^-$ are the creation and annihilation operators, respectively. The canonical variables $\hat{q}$, $\hat{p}$ corresponding to the frequency of the harmonic oscillator, therefore, the Hamiltonian of oscillator exciton system equation (5) is represented as:

$$\left(\frac{\hat{P}^2}{2}-4\mu^*\hat{q}^2\left[\frac{e^2}{4\pi\varepsilon_r\hat{q}^2}+E(\mu^*)\right]\right)\psi(q)=0\Rightarrow$$

$$\varepsilon_0(E.\omega.\mu^*)=\frac{\mathcal{D}}{4}\omega-\mu^*\frac{e^2}{4\pi\varepsilon_r}-2\mu^*\frac{\mathcal{D}}{\omega}E(\mu^*)=0 \quad (7)$$

where $\alpha_s=\frac{e^2}{4\pi}$ is the running coupling constant. Now stand on oscillator conditions $\varepsilon_0(E.\omega.\mu^*)=0$ and $\omega\frac{d\varepsilon_0(E.\omega.\mu^*)}{d\omega}=0$, one can define the minimum ground state energy of the exciton system as a result of the zero approximation (see Ref. [5] for more details). Therefore, the mass of exciton bound state in the 2D-TMDCM materials, oscillator frequency ω, reduced mass μ, energy eigenvalue $E(\mu)$ of the ground, and radial excitations states are defined in ORM using the following equation:

$$E(\mu^*)=\frac{\omega^2}{8\mu^*}-\frac{e^2\omega}{2\mathcal{D}\pi\varepsilon_r},\qquad \omega=\frac{2e^2}{\mathcal{D}\pi\varepsilon_r}\mu^* \quad (8)$$

And the steepest descent point method, the exciton bound state relativistic mass is defined as [7]:

$$M=\sqrt{m_e^{*2}-2\mu^{*2}\frac{dE(\mu)}{d\mu}}+\sqrt{m_h^{*2}-2\mu^{*2}\frac{dE(\mu)}{d\mu^*}}+\mu^*\frac{dE(\mu^*)}{d\mu^*}+E(\mu^*)=\sqrt{m_e^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2}+\sqrt{m_h^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2}-\mu^*\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2 \quad (9)$$

And the relativistic constituent masses of hole and electron read as:

$$\mu_e=\sqrt{m_e^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2},\ \mu_h=\sqrt{m_h^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2} \quad (10)$$

The reduced mass of exciton bound state is determined by the following equation [7]:

$$\frac{1}{\mu}=\frac{1}{\sqrt{m_e^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2}}+\frac{1}{\sqrt{m_h^{*2}+\mu^{*2}\left(\frac{e^2}{\mathcal{D}\pi\varepsilon_r}\right)^2}} \quad (11)$$

The bound state mass and the effective constituent masses of electron and hole in the exciton bound state (masses of constituent particles) are determined from equations (9) and (10), respectively. Now I apply results to determine the characteristics of the bound states defining exciton with the effective masses and dielectric constant $\varepsilon_{r\parallel},\varepsilon_{r\perp}$ (all essential taken data contained in Table 1). The numeric results are presented in Table 2. It is clear from Table 2, that the effective constituent mass of an electron and a hole differ from the masses in a free state and differ from effective masses (constituent mass of particles are larger). The mechanism for arising of the effective constituent mass of the relativistic exciton bound state forming electron and hole is explained in (9) by taking into account relativistic corrections. In Table 2, I also reported the ground state mass of exciton obtained theoretically through relativistic corrections. For example, our results for the mass of 2D-TMDCM materials such as 2H-MoS_2, 2H-WS_2, and 1T-HfS_2 are 0.146, 0.356, and 0.950, respectively, while their experimental values given in [12] are: 0.14, 0.11, and 0.39.

Table 1. The effective masses (in units of MeV), in-plane $\varepsilon_{r\parallel}$ and out-of-plane $\varepsilon_{r\perp}$dielectric constant or relative permittivity ($\varepsilon_r = \frac{\varepsilon}{\varepsilon_0}$) of 2D-TMDCM [11, 12].

1L TMDCMs	Effective mass ($\mathbf{MeV}$)		$\boldsymbol{\varepsilon_r}$	
	$\mathbf{m_e^*}$	$\mathbf{m_h^*}$	$\boldsymbol{\varepsilon_{r\perp}}$	$\boldsymbol{\varepsilon_{r\|\|}}$
2H-MoS2	0.55	0.56	6.4	15.1
2H-MoSe2	0.49	0.61	7.4	16.5
2H-MoTe2	0.65	0.64	8.8	19.5
2H-WS2	0.46	0.42	6.3	13.6
2H-WSe2	0.48	0.44	7.5	15.1
1T-HfS2	1.4	0.63	5.6	10.2
1T-HfSe2	1.8	0.51	6.7	13.9

Table 2. Mass spectra M(in units of MeV), the constituent effective mass of an electron μ_e^* and a hole μ_h^* of 2D-TMDCM materials: MX_2 QDs corresponding to the in-plane/out-plane $\varepsilon_{r||}/\varepsilon_{r\perp}$ dielectric constant

2D-TMDCM ($\boldsymbol{MeV}$)	$\boldsymbol{\varepsilon_{r\|\|}}$				$\boldsymbol{\varepsilon_{r_\perp}}$		
	$\boldsymbol{\mu_e}$	$\boldsymbol{\mu_h}$	$\boldsymbol{M}$	$\boldsymbol{M}$[12,13]	$\boldsymbol{\mu_e}$	$\boldsymbol{\mu_h}$	$\boldsymbol{M}$
2H-MoS2	0.384	0.388	0.416	0.14	0.293	0.298	0.543
2H-MoSe2	0.395	0.437	0.378	0.13	0.264	0.323	0.531
2H-MoTe2	0.677	0.675	0.322	0.16	0.362	0.357	0.605
2H-WS2	0.295	0.279	0.356	0.11	0.246	0.226	0.431
2H-WSe2	0.330	0.315	0.345	0.11	0.261	0.242	0.443
1T-HfS2	0.795	0.473	0.950	0.39	0.751	0.394	1.030
1T-HfSe2	1.065	0.596	0.990	0.49	0.982	0.431	1.206

4. Relativistic bohr radius of exciton

To calculate the relativistic radius of the exotic system with the circular orbits of a hydrogenic atom; i follow the ORM based on the approach used by Bohr for the nonrelativistic systems. The Coulomb type potential with the electrostatic field of attraction between the electron and nuclear core, intended as $F_c = -\nabla U$ must equal $-\nabla U = mr^3\varpi^2$, by performing Bohr energy and Coulomb potential, I obtain the Bohr radius for hydrogen-like atom: $r_B = \frac{4\pi}{e^2 m_e} n^2 \cong 0.053nm$. n is the principal quantum number. I can construct a nonrelativistic Bohr model for an exotic exciton system. As far as we know, the motion of the exciton in the QDs has a relativistic behavior, and one of the motivations for theoretically studying exciton is to determine the relativistic Bohr radius without using and the relativistic kinetic energy and the Dirac model. Using the relativistic kinetic energy with the Bohr quantization rule, I can determine the relativistic radius of the orbit [13]:

$$r_B^{rel} = \frac{1}{1+\gamma}\frac{8\pi}{e^2 m_e} n^2 = \frac{2}{1+\gamma} r_B < r_B \quad (14)$$

where $\gamma \geq 1$ is the Laurence factor. The next step is to determine the exciton Bohr radius systems in the 2D-TMDCM QDs materials. Bohr radius of exciton describes the relative distance between electron/hole particles and has a pronounce on the properties of the exotic system. In the experimental aspect, the exciton Bohr radius in 2D-TMDCM materials was determined and it is several times larger than the theoretical methods. In this section, I investigate the exciton Bohr radius in 2D-TMDCM materials with a

strong Coulomb coupling constant $\alpha_s \approx 0.09$ in the framework of ORM. The exciton Bohr radius formula reads: $r_{exc} = \frac{m_e \varepsilon_r}{m^*} n^2 r_B$. Where m^* is the nonrelativistic reduced mass of the exciton system. From the previous section, the exciton Bohr radius with effective masses of electron and hole in 2D-TMDCM materials reads as follows:

$$r_{exc} = \frac{m_e^* m_h^*}{m_e^* + m_h^*} m_e \varepsilon_r n^2 r_B \quad (15)$$

Using the (15) and (10), the relativistic exciton Bohr radius is defined as [13]:

$$r_{exc}^{rel} = \frac{m_e}{\mu^*} \varepsilon_r n^2 r_B = \frac{\mu_e^* \mu_h^*}{\mu_e^* + \mu_h^*} m_e \varepsilon_r n^2 r_B \quad (16)$$

Here without loss of generality, the relativistic Bohr radius may be set equal to nonrelativistic ($r_B \cong r_B^{rel}$) for convenience. Exotic Bohr radius with heavy/light hole in monolayer, bilayer, and multilayer QDs materials are currently fascinating subjects in SQDs physics. Therefore, i calculate the relativistic Bohr radius of circular orbits of an exotic exciton, and the numeric results are presented in Table 3. The mechanisms of contraction in the exciton Bohr radius are explained in (10). According to the relativistic theory of space-time and the relativistic equation (10), the exciton Bohr radius is more contracted than that of the classical exciton Bohr radius. The result is consistent with the fact that the absolute value of relativistic energy of exciton (i.e., an electron in the exciton system) is more positive than a nonrelativistic one.

Table 3. The relativistic r_{exc}^{rel} (in units of nm) and nonrelativistic r_{exc} Bohr radius (in units of nm) of exciton in 2D-TMDCM materials: MX2 QDs corresponding to the in-plane/out-plane $\varepsilon_{r||}/\varepsilon_{r\perp}$ dielectric constant

2D-TMDCM materials	$\boldsymbol{\varepsilon_{r\|\|}}$		$\boldsymbol{\varepsilon_{\perp}}$	
	$\boldsymbol{r_{exc}^{rel}}$	$\boldsymbol{r_{exc}}$	$\boldsymbol{r_{exc}^{rel}}$	$\boldsymbol{r_{exc}}$
2H-MoS2	2.115	2.880	1.170	1.221
2H-MoSe2	2.151	3.213	1.378	1.441
2H-MoTe2	1.552	3.183	1.324	1.444
2H-WS2	2.567	3.278	1.447	1.519
2H-WSe2	2.534	3.481	1.615	1.729
1T-HfS2	0.930	1.242	0.586	0.682
1T-HfSe2	0.983	1.851	0.605	0.892

The electron is more bound to the quasiparticle, then the exciton Bohr radius must be smaller than the nonrelativistic exciton radius, but for exciton velocity much less than the speed of light in semiconductors, the relativistic radius tends to that of classical radius. In Table 3, i determined the relativistic Bohr radius of the exciton. For example, our results for the 2H-MoS_2, 2H-WS_2, and 1T-HfS_2 are 2.567 and 0.930, respectively, while the nonrelativistic values are: 2.88, 3.278, and 1.851.

5. EXciton wave function

Now, let's formulate the ground state wave function in the 2D-TMDCM materials. As we know, the wave function of the ground state of an exotic atom in terms of ORM has the form [5]:

$$|\Psi_0\rangle = \prod_{i=1}^{D} \left(\frac{\mu^* \omega_0}{\pi}\right)^{\frac{\mathcal{D}}{4}} e^{-\frac{\mu^* \omega_0}{2} q_i^2} \quad (17)$$

In the particular case $\ell = 0$, we have the axillary space $\mathcal{D} = 4$, and $\omega_0 = \frac{e^2}{2\pi\varepsilon_r}\mu^*$, then the ground state wave function reads

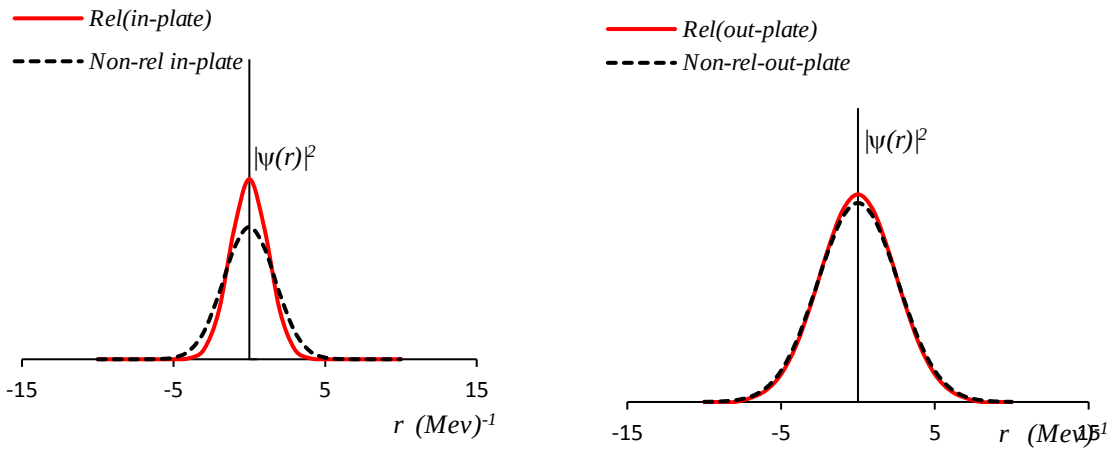

Fig. 3. Probability density of exciton in a monolayer 2H-MoS_2 versus r. With and without the relativistic effective mass of exciton corresponding to the in-plate $\varepsilon_{r||}$ (left) and to the out-plate $\varepsilon_{r\perp}$ (right) directions of dielectric constant.

$$|\Psi_0\rangle = \left(\frac{\mu^*\omega_0}{\pi}\right) e^{-\frac{\mu^*\omega_0}{2}q^2} \quad (18)$$

And satisfies the well-known conditions $\langle\Psi_0|\Psi_0\rangle = 1$ and $\hat{a}^-|\Psi_0\rangle = 0$. All radial excited states $\ell \neq 0$ can be determined by $|\Psi_\ell\rangle = (\hat{a}^+\hat{a}^+)^\ell|\Psi_0\rangle$. I study the wave function of excitons in the 2D-TMDCM materials and consider for 2H-MoS_2 with $\ell = 0$, using ORM. In Fig. 1, the behaviors of the radial wave functions of exciton with the relativistic and nonrelativistic effective mass of an electron and a hole in different directions in the monolayer 2H-MoS_2 are plotted. The probability density in Figure 3, is given by taking the μ^* and m^* values in the exciton wave function: $|\Psi_0\rangle_{rel} = \left(\frac{\mu^*\omega_0}{\pi}\right) e^{-\frac{\mu^*\omega_0}{2}q^2}$, $|\Psi_0\rangle_{nonrel} = \left(\frac{m^*\omega_0}{\pi}\right) e^{-\frac{m^*\omega_0}{2}q^2}$. The plot gives us the likelihood of finding an exciton system in the monolayer 2H-MoS_2 with $|\Psi_0\rangle_{rel}$ is than $|\Psi_0\rangle_{nonrel}$ and shows that the amount of energy carried by a wave function is related to the amplitude of the $|\Psi_0\rangle_{rel}$. The amplitude of relativistic wave function $|\Psi_0\rangle_{rel}$ is larger than$|\Psi_0\rangle_{nonrel}$, i.e., an exciton system in the monolayer 2H-MoS_2 with relativistic effective masses has a higher amount of displacement than the other one (with nonrelativistic effective masses).

6. Results and discussion

Exciton parameters have been studied in higher energy interactions than Coulomb potential and bandgap using several theoretical and experimental models. The present paper proposed a method for theoretically determining the relativistic exciton Bohr radius, relativistic mass, and energy eigenvalue of the ground state within the framework of the QFT, QED. An analytic expression was given for masses of exotic systems while considering relativistic corrections. I computed the masses and energy of charged/quasi-charged bound states by considering the system as a hole core and electron. I have theoretically investigated the features of the exciton Bohr radius of charge carriers in the 2D-TMDCM materials. The calculation was performed using the bound state method to solve the Schrödinger equation for the exciton system. In the Radial Schrödinger equation, the Wick-ordering method called ORM is proposed to calculate the mass spectrum and relativistic Bohr radius of the exciton system in the 2D-TMDCM materials for an electrostatic potential allowing the existence of an electron-hole bound state. I have calculated the relativistic exciton Bohr radius values for free and pure 2D-TMDCM materials corresponding to the in-plane and out-of-plane directions. I have considered 2D-TMDCM materials: molybdenum (Mo), tungsten (W), hafnium (Hf) based on 2D-TMDCM materials. The motivation for this research comes from a recent report on the practical realization of excitons in 2D-TMDCM materials. In this context, I present the calculated electron-hole relativistic radius and relativistic mass spectrum. Quantitative characterization of bound state constituent effective mass of the electron-hole, via the corresponding charged current in QFT is given. I have calculated and determined the theoretical value for the ground state wave function of the exciton in 2D-TMDCM systems. The wave function of bound states that can be achieved in the SQDs is important and may provide potential applications in quantum information processing, excitonic solar cells, electro-photo catalysts, super batteries-capacitors, and also the characteristics of exciton in SQDs studied. I have defined that the in-plane dielectric relativistic Bohr radius is smaller than the out-of-plane dielectric response for all the 2D-TMDCM materials, and it is

smaller than the nonrelativistic Bohr radius. The calculated exciton Bohr radius, the mass spectrum, effective constituent masses of the electron, and hole parameters for ORM are provided in Table 2 and Table 3.

As expected, Table 3 shows that the exciton Bohr radius of the exciton system decreases. That opens the door to even more applications in quantum information technology on a quantum level. In Table 2 and Table 3, i have described the relationship of the exciton mass and exciton Bohr radius in the 2D-TMDCM materials, without spin-spin or spin-orbital interactions. This result could revolutionize the way engineers approach electronics. It can be concluded that theoretical results can help scientists to study excitons' extraordinary properties in order to design more energy-efficient electronic systems and find a way to better control excitons moving in semiconductors, Ultrafast THz spectroscopy, and Magneto-Optical Investigation, and Ultrafast THz spectroscopy, Magneto-Optical investigation, and Ultrafast optical spectroscopy. Also, they can find a new way to polarize the exciton currents in higher energies.

7. Conclusion

I have studied exciton in the 2D-TMDCM materials under the electrostatic field. The energy eigenvalue, the frequency, and effective relativistic masses of the exciton are established and calculated in the framework of the oscillator representation method. This result leads us to conclude that the behavior of the exciton, can be modeled by QFT as a particle/quasiparticle bound state. The investigation may become an invaluable help in electronic devices and quantum information processing based on the SQDs materials. I determined the ground state relativistic Bohr radius of exciton which is inside the 2D-TMDCM materials: MX_2 QDs materials using the oscillator representation method, the effective mass, and considering a hydrogenic wave function for the ground state. I take into account the presence of relativistic Bohr radius and effective constituent masses dependent on the electron-hole relativistic motion and direction of the dielectric constant. The results may be resumed thus: (i) the relativistic behavior of electron-hole motion in the 2D-TMDCM materials decreases the exciton Bohr radius for all MX_2 in QDs materials. (ii) the effective relativistic mass of the exciton system is larger than the nonrelativistic effective mass. (iii) the amplitude of relativistic wave function $|\Psi_0\rangle_{\mathrm{rel}}$ is larger than $|\Psi_0\rangle_{\mathrm{nonrel}}$. I hope that these results will motivate future experimental work in this direction that will confirm my predictions.

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