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Research paper

Exciton properties in 2D-Xenes nanomaterials within quantum field approaches

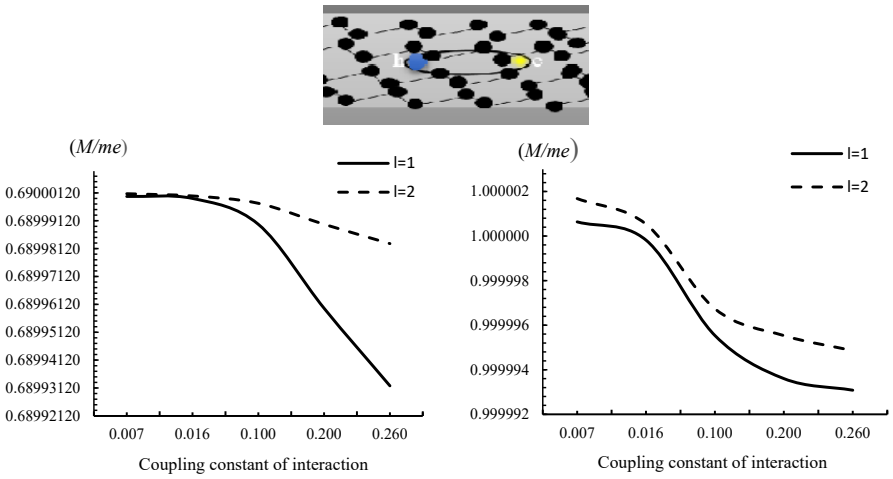
Arezu Jahanshir

Department of Physics and Engineering Sciences, Buein Zahra Technical University, Buein Zahra, Iran

HIGHLIGHTS

- Considering gas catalysis tautomerism.
- Applying Carmustine as anti-cancer drug.
- Applied DFT method for considering drug behavior.
- Use different basis sets for analysis.
- Calculation of thermodynamic energy of tautomerism.

GRAPHICAL ABSTRACT



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ABSTRACT

There have been substantial theoretical advances in the field of condensed matter physics in recent years. These significant developments have spanned many different principles. For example, accelerated research into understanding how quantum field theory is connected to physics has attracted a lot of attention from other domains. In particular, exciton and magnetoexciton coupled systems are popular due to their compatibility with experimental research. This study investigated and presented a theoretical description of electron-hole–photon interactions and excitonization in a microcavity nano-quantum environment based on QED, QFT, and quanto-relativistic behavior of the electron-hole coupled system. This work represents conversion, a main theoretical and applied physics subject, including electronic technologies, electro-photo catalysts, super batteries capacitors, qubits, quantum computation, and magneto-excitonic solar cells. The quanto-relativistic mass and the coupled electron-hole systems were investigated using the Rytova-Keldysh and Coulomb potential in a free exciton system. The ground and excited coupled state energy and mass of free exciton as an atomic system in the oscillator explanation of a symplectic group were determined. This projective method is in line with other theoretical methods and could be useful to study and predicate several different multi-excitons exotic systems and determine the angular velocity of exotic coupled states and relativistic mass of particles, which is important in mono elemental or non-mono elemental nanolayers materials.

* *Corresponding author: Tel.: +9828-33894493 ; Fax: +9828-33894493 ; E-mail address: jahanshir@bzte.ac.ir*
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1. Introduction and methodology

In this study, we describe mono elemental nanolayers (MEM), like Ge Fs (Germanene), Sn Fs (Stanene), and Si Fs (Silicene), Graphene-like structures, the masses of electrons and holes equal $m_e^* = m_h^*$, and non-mono elementals (NMEM), like Ge Se, Ga As, In P, and MoS_2. Fs refers to the freestanding monolayers (monolayers in a vacuum). As we know, elemental graphene-like 2D materials are called Xenes, where X refers to group-IV, group-V, or group-VI elements, which possess electronic properties different from those of the corresponding 3D materials. These structures have the potential to open new nanoscale research frontiers in science and nanotechnology. This structure has different properties that make mono elemental nanolayers a possible candidate for the next generation of high technologies materials. Magnetoexciton is an electrically neutral exotic quasiparticle that exists in all mono elemental nanolayers. Magnetoexciton is bounded by a negatively charged electron and a positively charged hole that are attracted to each other by the electrostatic Coulomb interaction. The experimental discovery of exotic magnetoexcitons in nano-quantum layer levels has been expanded into the potential for the experimental existence of multi-exciton states, and considerable interest has been directed toward these multi-exciton state properties, especially the related state in direct and indirect orientation.

Magnetoexcitons, as exciting oscillating quantum systems, are described by various potential models. The Rytova-Keldysh (RK) potential has been presented for direct magnetoexciton orientation and the Coulomb potential for indirect magnetoexciton orientation. In this paper, the RK potential was used to describe electrostatic interaction between particles and was expressed as Eq. (1).

$$V_{RK}(r,T) = -\frac{q^2}{8r_0\varepsilon(T)\varepsilon_0\left(\frac{\varepsilon_{1(T)}+\varepsilon_{2(T)}}{2}\right)}\left(H_0\left(\frac{r+D}{r_0}\right) - Y_0\left(\frac{r+D}{r_0}\right)\right) \quad (1)$$

where Y_0 and H_0 are the zeroth order of Bessel and Struve functions, ε_1 and ε_2 are the material's dielectric constants, ε is surrounded by an environment above and below with permittivity's $\varepsilon_1, \varepsilon_2, r_0$ is the screening length proportional to the polarizability of mono elemental nanolayers $r_0 = 0.5\ \varepsilon l\ (\varepsilon_1 + \varepsilon_2)^{-1}$, l is the thickness of the layer, and D is the interlayers separated distance. This type of potential adequately describes the interaction and can be used in determining the potential of interaction between multi-particle electron-hole bound states in metal or nano-quantum layers. Using the RK potentials, one can determine the mass spectrum and eigenenergies of the magnetoexciton bound state. The mass is suggested based on the Gaussian behavior field parameters in the exotic coupled system [1,2,3]. Thus, the parameters for the ground states can be established using the RK potential in the procedure of a projective unitary representation of the symplectic group and the projective unitary representation (PUR) or oscillator explanation method [1].

The magnetoexciton coupled state is a hydrogen-like atom, so nonrelativistic potential models can be used to study it. Our findings show that the component hole-electron masses differ from the other masses of the particles. The constituent mass of the hole is relatively greater than the electron, and the electron-hole constituent masses in the quantum dot plates differ from the electron-hole of other structures. In this study, the ground-coupled states of electron-hole were determined. While the radial Schrödinger equation (RSE) analytically and precisely predicts the probability of events or outcomes, it does not produce solutions, so several different numerical approximations and theoretical principles have been developed. The magnetoexciton system's associated, operator creation, and annihilation principles were proposed to determine the rotational velocity of a coupled state as a function of the orbital quantum number, which consists of an electron and a hole. The rotational velocity is the main variable describing the interaction between coupled electron-holes that create bounding states like a proton-electron, electron-positron, *etc*. With the help of QFT and QED theories, we find that the creation of a related state occurs if the gauge boson masses and the coupling constant of interaction are very small with regard to the constituent particulate masses.

In this article, we show how a modified Hamiltonian (Schrödinger equation) based on the PUR and using the angular velocity of coupled state can be used to describe the characteristics (*i.e.*, the mass spectrum, the constituent mass of an electron-hole, and eigenenergy) of the coupled state. The technique is characteristically used to determine and solve a relativistic or nonrelativistic Schrödinger equation and to calculate the eigenenergy or bounding energy of the coupled electron-hole system

for an RK potential. The main goal of this study is to use the nonrelativistic Schrödinger equation to investigate the relationship of the electron-hole eigenenergy with the rotational velocity of the coupled state. First, a theoretical description of the electron/hole effective mass based on relativistic characteristics of interaction or the quanto-relativistic behavior of exotic magnetoexciton bound state is presented. Then, using this method, we demonstrate the projective unitary representation of the symplectic group while calculating the energy levels and coupled mass of magnetoexcitons [3]. Since the characteristics of magnetoexcitons can be accurately described by PUR, it is important to develop the PUR in nano-quantum physics, as it describes the coupled-state features and specifications of quasi-atom states. Next, the RSE is performed for the RK potential, and the coupled state of electron-hole eigenvalue is calculated for the ground stats and excited states. Finally, the single magnetoexciton energy levels under the average gauge field are presented.

2. Quantum field theory framework

A variety of quasi-particles with relativistic characteristics can be found in condensed matter, semiconductor materials, thin-film, and mono elemental nanolayers. In particular, semiconductors can sustain bound electron-hole (e-h) pairs and exotic bound states (magnetoexcitons). Electron-holes in semiconductors and other specific materials behave like bound states or bosonic states and can be presented as a Bose-Einstein condensate at very low temperature (as 1 to 10K); they behave very differently at very high temperatures (200 to 370K). Magnetoexciton behavior, as a Bose-Einstein condensate state, was described theoretically in 1962 [4-7]. The realization of magnetoexciton's new characteristics in semiconductors and high-tech materials would open new opportunities in the manipulation of quantum properties because of the greater flexibility and well-developed technology of semiconductor and 2D materials. In this article, the mass of the coupled-state is defined by the infinite-asymptote action of the correlation function (CF) of the particle currents with specific characteristics like quantum numbers. Based on Green's function, the CF is represented as a functional Feynman path integral (FFPI), which allows us to describe the infinite-asymptote action. Hence, we can average it over the external field. The resulting method in nonrelativistic quantum mechanics is very close to the FFPI. In this case, the interaction potential can be determined by the Feynman diagram, and the constituent mass of the particle in the coupled-state differs from the initial mass state. Thus, the constituent mass gives us relativistic corrections to the Hamiltonian of interaction. The details of this approach are briefly discussed below.

The magnetoexciton bound state is a quasi-exotic state explained by the confining potential within the coupling constants of interaction. The magnetoexciton bound state can be described and its specifications defined at a finite temperature [8,9] using the modified radial Schrödinger equation [8]. Therefore, in this present work, we considered a system consisting of the main state and the radial excited states of the magnetoexciton bound state. This method should be considered a good approximation to the more excited states. The bound state equations and mathematical descriptions in nonrelativistic quantum mechanics are similar to the Feynman functional path integral. Hence, the mass of coupled electron-hole can be determined by the polarization function (statistical correlation) $\Pi(r)$ and Green's function $G(r)$ [1]. Since Green's function is described in a functional integral form, the coupled electron-hole mass spectrum should be explained in relativistic quantum theory in the following relations [9,10].

$$M = -lim_{|r|\to\infty}|r|ln\Pi(r) = -lim|r|ln(\langle G_1(r)|G_2(r)\rangle) \qquad (2)$$

$$= \int\int A d\mu_1\, d\mu_2 e^{-\frac{1}{2}\int d\xi B(\alpha\mu_1-\beta\mu_2)-V(r)} e^{-\frac{1}{2}rV(r)[(\mu_1 m_1^2+\mu_1{}^{-1})+(\mu_2 m_2^2+\mu_2{}^{-1})]} =$$

$$= \int\int A d\mu_1\, d\mu_2 e^{-rE(\mu_1,\mu_2)} e^{-0.5rV(r)[(\mu_1 m_1^2+\mu_1{}^{-1})+(\mu_2 m_2^2+\mu_2{}^{-1})]} =$$

$$= \frac{\partial}{\partial\mu_1,\mu_2}\left(\frac{1}{2}(\mu_1{}^{-1}m_1^2+\mu_1{}^{-1})+\frac{1}{2}(\mu_2{}^{-1}m_2^2+\mu_2{}^{-1})+E(\mu_1,\mu_2)\right) =$$

$$= \frac{\partial}{\partial\mu_1,\mu_2}\left(\left(\frac{\mu_2 m_1^2+\mu_1 m_2^2}{2\mu_1\mu_2}\right)+\frac{1}{2}\mu+E(\mu)\right)$$

where asymptotic of the function $\Pi(r)$ for n-body system is:

$$\boldsymbol{\Pi}(x) = \int_0^{\infty}\int_0^{\infty}\ldots\int_0^{\infty}\frac{1}{(8x\pi^2)^n}\prod_{i=1}^{n}d\mu_i\,.\,\boldsymbol{exp}\left\{\sum_{i=1}^{n}-\frac{|x|}{2}\left(\frac{m_i^2}{\mu_i}+\mu_i\right)\right\}\prod_{i=1}^{n}N_i\int\int\ldots\int\prod_{i=1}^{n}\delta r_i\times$$
$$\boldsymbol{exp}\left(-\frac{1}{2}\int d\tau(\textstyle\sum_{i=1}^{n}\mu_i\dot{r}_i(\tau)\ )\right).\boldsymbol{exp}\left(-\textstyle\sum_{i=j=1}^{i=j=n}W_{ij}+2\sum_{i,j=1,i\neq j}^{n}W_{ij}\right) \qquad (3)$$

Then, the coupled state mass in the stationary state reads as:

$$M = \frac{\partial}{\partial \mu_1, \mu_2}\left(\frac{\mu_1 m_2^2 + \mu_2 m_1^2}{2\mu_1\mu_2} + \frac{\mu}{2} + E(\mu)\right) \quad (4)$$

where μ is the reduced mass defined by:

$$\mu = \frac{\mu_1\mu_2}{\mu_1+\mu_2} \quad (5)$$

and using the Taylor approximation, one can determine parameters $\mu_{i\,(i=1,2)}$ as follows [10]:

$$\mu_1 = \frac{\partial M}{\partial \mu_1} = \frac{\partial E(\mu)}{\partial \mu_1}\mu_1 + \frac{1}{2}\mu_1 - \frac{1}{2}\frac{m_1^2}{\mu_1} = 0 \Rightarrow \mu_1 = \left(m_1^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{\frac{1}{2}} \quad (6)$$

and:

$$\mu_2 = \frac{\partial M}{\partial \mu_2} = \frac{\partial E(\mu)}{\partial \mu_2}\mu_2 + \frac{1}{2}\mu_2 - \frac{1}{2}\frac{m_2^2}{\mu_2} = 0 \Rightarrow \mu_2 = \left(m_2^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{\frac{1}{2}} \quad (7)$$

with the binding energy E_{bin} calculated below:

$$E_{bin} = \left(m_1^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2} + \left(m_2^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2} + \mu\frac{dE(\mu)}{d\mu} + E(\mu) - (m_1 + m_2) \quad (8)$$

where μ is the reduced mass of the system, m_1 and m_2 are the free particle mass (rest mass), μ_1 and μ_2 are the constituent masses of the particle in the bound state, and we consider that m_1 and m_2 in the magnetoexciton system equivalent to the effective masses m_e^* and m_h^*.

3. Relativistic correction of Schrödinger equation

The magnetoexciton is a quasi-exotic state in both the hole and electron relativistically. Therefore, the magnetoexciton bound state at a finite temperature in the mono elemental nanolayers can be specified using the Schrödinger equation, which enabled us to describe and define magnetoexciton specifications. We can explain bound state interactions based on the modified Schrödinger equation with relativistic correction, according to the projective unitary representation (PUR) at finite temperature, using Eqs. (6)-(8) for two particles in a bounded state [10-12]. Therefore, we can also explain the relativistic effect on the bound states using explanations *I* and *II* as Eq. (9) (based on the saddle point method or the method of steepest [10]) according to the equations and ideas in the above paragraph.

$$\begin{aligned} &I.\ \sqrt{m^2 + \hat{p}_r^2} = m\sqrt{1 + \frac{\hat{p}_r^2}{m^2}} \approx m + \frac{\hat{p}_r^2}{2m} - \frac{\hat{p}_r^4}{8m^3} + \cdots \\ &II.\ \sqrt{m^2 + \hat{p}_r^2} \approx \min_{\mu}\frac{1}{2}\left(\mu + \frac{m^2+\hat{p}_r^2}{\mu}\right) \end{aligned} \quad (9)$$

Then Schrödinger's equation $\hat{H}\Psi = \varepsilon\Psi$ can be presented in a modified form (the radial relativistic Schrödinger equation):

$$\left(\sqrt{m_e^2 + \hat{p}_r^2} + \sqrt{m_h^2 + \hat{p}_r^2} + V(r,T)\right)R(r) = E(\mu^*)R(r) = 0 \quad (10)$$

where $|\hat{p}_e^{\,2}| = |\hat{p}_e^{\,2}| = |\hat{p}_r^{\,2}|$. This method is generally used to predict the structure of the bound states mass spectrum (M) and eigenenergy (ε); hence, the Hamiltonian of the magnetoexciton bound state with the potential interaction $V(\boldsymbol{r})$ between the hole is given by [10].

$$\begin{aligned} &\hat{H}\Psi = \varepsilon\Psi \Rightarrow \left[\frac{\hbar^2}{2}\left(\mu_e + \frac{m_e^2+\hat{p}_r^2}{\mu_e}\right) + \frac{\hbar^2}{2}\left(\mu_h + \frac{m_h^2+\hat{p}_r^2}{\mu_h}\right) + V(\boldsymbol{r})\right]\Psi = M\Psi \Rightarrow \\ &\left[\frac{\hbar^2}{2\mu}\hat{p}_r^2 + V(\boldsymbol{r})\right]\Psi = \left[M - \frac{\mu_e+\mu_h}{2} - \frac{m_e^2\mu_h + m_h^2\mu_e}{2\mu_e\mu_h}\right]\Psi \end{aligned} \quad (11)$$

$$\frac{1}{\mu} = \frac{1}{\left(m_e^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2}} + \frac{1}{\left(-2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2}} \quad (12)$$

where μ_e and μ_h are the constituent mass of components (electron and hole) in the bounding system, and μ is the reduced mass determined and presented in the above paragraph. By including spin orbit interactions, we can obtain the Hamiltonian and also determine the mass difference between the degenerate exotic magnetoexciton states. In mono elemental nanolayers, one can present the Hamiltonian of spin-spin and spin-orbit terms by applying an electric or magnetic field in a specific direction, like z, which couples with the spin of the electron and hole in nanomaterials. The Hamiltonian of spin orbits interactions is determined by Eq. (13).

$$\hat{H}_{spin\text{-}orbit} = \hat{H}_{SS} + \hat{H}_{LS} = \alpha\,(E(r) \times \hat{p}_r^{\,2}).\vec{\sigma}_i \quad (13)$$

where $\hat{p}_r^{\,2}$ is the momentum operator, α is the constant of spin-orbit interactions, and $\vec{\sigma}_i$ is the Pauli spin matrices. Spin-orbit coupling is the first-order portion of the relativistic effect in atoms or molecules. For simplicity, this refinement in the calculation has been ignored. In the relativistic-quantum field, the mass of the coupled particles is presented by the Gaussian shape of the correlated-current function and the exact orbital quantum numbers. In terms of Green's function, the statistical correlation is expressed and defined as a functional integral, allowing the necessary Gaussian limit to be allocated. Then, the average value of the external gauge field was calculated.

4. Magnetoexciton in 2D materials

The analytical solution for the Schrödinger equation was obtained for $V_{RK}(r,T)$ and $V_C(r,T)$ potentials at a finite temperature with the radius r ($0 \le r < \infty$), d-dimensional space, and angles (θ,φ). The Hamiltonian of an electron-hole coupled system (see Fig. 1(a)) (electron-hole coupled but a suggested free magnetoexciton system) [13,14] with momentum $\hat{p}$ and interaction potential reads as follows:

$$\hat{H}_{total}\Psi_n = \varepsilon(\mu)\Psi_n = \varepsilon(\mu)R(r)Y(\theta,\varphi) \tag{14}$$

$$\hat{H}_{total} = \hat{H} + \hat{H}_{spin}$$

The electron-hole bound system in the external uniform magnetic field within the interacting potential $V(r)$ and the spin-orbit interaction at finite temperature can be described by vector $\boldsymbol{A}$ or $\boldsymbol{B}$ by the Hamiltonian:

$$\hat{H} = \frac{1}{2m_e^*}\left[\hat{P}_e + \frac{q^2}{2c}[\boldsymbol{B}\times r_e]\right]^2 + \frac{1}{2m_h^*}\left[\hat{P}_h - \frac{q^2}{2c}[\boldsymbol{B}\times r_h]\right]^2 + V(r_{eh}) - g_L\mu_B(\boldsymbol{L}\cdot\boldsymbol{S}) + g_S\mu_B(\boldsymbol{S_e}+\boldsymbol{S_h})\cdot\boldsymbol{B}. \tag{15}$$

where $V(r_{eh})$ is the potential interaction and the vector potential $\boldsymbol{A} = \frac{q}{2c}[\boldsymbol{B}\times\boldsymbol{r}]$ of the system corresponding to the magnetic field $\boldsymbol{B}$ = (0, 0, B), which is presented perpendicular to the direction of the magnetoexciton $-\frac{iq}{m^*}(\boldsymbol{A}\cdot\nabla) = \frac{q}{2m^*}(\boldsymbol{B}\cdot\boldsymbol{L})$, $\frac{q^2}{2m^*}\boldsymbol{A}^2 = \frac{q^2}{2m^*}(\boldsymbol{B}\times\boldsymbol{r})^2$ are

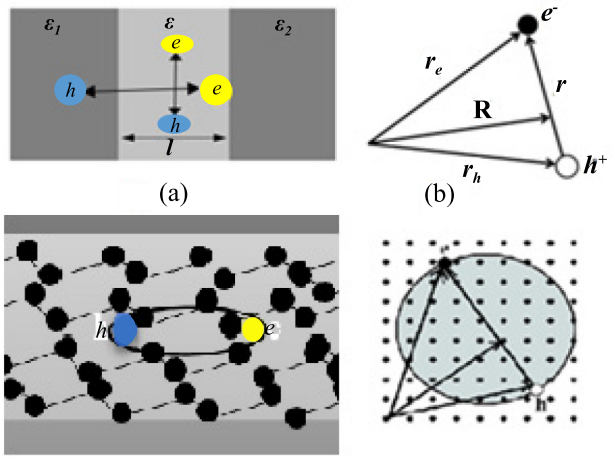

Fig. 1. The relative motion of the direct and indirect electron-hole bound state in mono elemental 2D nano-quantum materials. Where l is the nanosheet thickness, ε_1 and ε_2 are the electrical permittivity of the medium above and below the mono elemental nanolayers, and ε is the electrical primitivity of part surrounding the interlayers.

the effective mass of particles in the bound state under the magnetic field in the mono elemental 2D nano-quantum materials, m_e = 0.511 MeV is the rest mass of electrons, and m_h = 0 is the hole in the free state. Using Eqs. (6) to (8) and ignoring the spin-orbit interaction, using Eq. (9), we have:

$$\hat{H} = \left[-\frac{\hbar^2}{2m_e^*}\Delta_e - \frac{\hbar^2}{2m_h^*}\Delta_h + \frac{q^2}{8m_e^*}\boldsymbol{A}^2 + \frac{q^2}{8m_h^*}\boldsymbol{A}^2 + \frac{iq}{cm_e^*}(\boldsymbol{A}\cdot\nabla) + \frac{iq}{cm_h^*}(\boldsymbol{A}\cdot\nabla)\right] + V(r) \tag{16}$$

We can present and investigate the exciton Bohr radius in 2D-Xene nanomaterials and define the relation between the lattice constant and the exciton Bohr radius with a well-known Coulomb coupling constant in the framework of quantum mechanics [16]. First, the exciton Bohr radius formula reads $r_{exc} = \frac{m_e\varepsilon_r}{m^*}n^2r_B$, where m^* is the nonrelativistic reduced mass of the exciton system. Then, the exciton Bohr radius with effective masses of the electron and hole can determine by $r_{exc} = \frac{m_e^*m_h^*}{m_e^*+m_h^*}m_e\varepsilon_r n^2 r_B$. Next, we can define the lattice constant and its relation to the atomic radii for each monoelemental material; then, using this formula, we can present the nanomaterial properties of the electron-hole characteristics. Now, one can present Eq. (9) under the Jacobian coordinate transformation of the electron-hole bound state in mono elemental nanolayers (see Fig. 1(b)). The Jacobi coordinates based on Fig. 1(b) of the magnetoexciton system are:

$$r_e = \frac{m_h^*}{M}\boldsymbol{r} + \boldsymbol{R}$$

$$r_h = \frac{m_e^*}{M}\boldsymbol{r} + \boldsymbol{R} \tag{17}$$

$$M = m_e^* + m_h^*$$

where $\boldsymbol{r}$ is the vector of relative motion and R is the vector of the center of mass. The total Hamiltonians of the magnetoexciton $\hat{H}\Psi = \varepsilon\Psi$ is defined as:

$$H = -\frac{\hbar^2}{2M}\Delta_R - \frac{\hbar^2}{2\mu^*}\Delta_r + \frac{q^2}{8\mu^*}(\boldsymbol{B}\times\boldsymbol{R})^2 + \frac{\mu^{*2}q^2}{8\tilde{\mu}}(\boldsymbol{B}\times\boldsymbol{r})^2 - \frac{iq}{2M}(\boldsymbol{B}\times\boldsymbol{r})\cdot\nabla_R - \frac{iq}{2\mu^*}(\boldsymbol{B}\times\boldsymbol{R})\cdot\nabla_r - \frac{iq\gamma}{2\mu^*}(\boldsymbol{B}\times\boldsymbol{r})\cdot\nabla_r + \frac{\gamma q^2}{4\mu^*}(\boldsymbol{B}\times\boldsymbol{r})\cdot(\boldsymbol{B}\times\boldsymbol{r}) + V(\boldsymbol{r}) \tag{18}$$

where

$$\frac{1}{\tilde{\mu}} = \left(\frac{1}{m_e^{*3}} + \frac{1}{m_h^{*3}}\right),\quad \gamma = \frac{m_h^*-m_e^*}{m_e^*+m_h^*},\quad \mu^* = \frac{m_e^*\cdot\mu_h^*}{m_e^*+m_h^*},\quad M = m_e^* + m_h^*.$$

We describe Eq. (11) based on the relative motion (specified, r) for the bound state of electron and hole with zero centers of mass momentum (specified, R),

and also consider the wave function of the electron-hole bound state in the magnetic field as shown by the modified wave function $\varphi(r,R)$:

$$\Psi_n \to \varphi(\boldsymbol{r}.\boldsymbol{R}) = \phi_0\left(\boldsymbol{r} - \frac{1}{q\boldsymbol{B}^2}(\boldsymbol{B}\times\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]\right)\times \quad (19)$$
$$exp\left(i\boldsymbol{R}\cdot(\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right] + \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right).exp\left(\frac{iy}{2}\left(\boldsymbol{r}\cdot\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]\right)\right)$$

Based on the properties of mono elemental 2D nano-quantum materials, the masses of electrons and holes are equal $m_e^* = m_h^* = m^*$, so we can rewrite Eq. (11) by affecting the wave function on the Hamiltonian $H\varphi\,(r,R) = \varepsilon(\mu)\,R(r)\,\phi(R)$ and using, $\mu^* = \frac{m^*}{2}.\frac{1}{\tilde{\mu}} = \frac{2}{m^{*3}}$, $\gamma = 0$. Then, the relative Hamiltonian H_r in these variables can be defined as:

$$H_r = -\frac{\hbar^2}{2\mu^*}\Delta_r + \frac{1}{8\mu^*}\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]^2 + \frac{q}{4\mu^*}\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]\cdot(\boldsymbol{B}\times\boldsymbol{r}) + \frac{q^2}{8\mu^*}(\boldsymbol{B}\times\boldsymbol{R})^2 - \frac{iq}{2\mu^*}(\boldsymbol{B}\times\boldsymbol{R})\cdot\nabla_r + V(\boldsymbol{r}) \quad (20)$$

and, the n dimensional Schrödinger equation for the radial function is:

$$\left(-\frac{\hbar^2}{2\mu^*\boldsymbol{r}^n}\frac{d}{d\boldsymbol{r}}\left[\boldsymbol{r}^{n-1}\frac{d}{d\boldsymbol{r}}\right] - \frac{\hat{\boldsymbol{L}}^2}{2\mu^*\boldsymbol{r}^2} + V(\boldsymbol{r})\right)\varphi(\boldsymbol{r},\boldsymbol{R}) = E(\mu^*)\varphi(\boldsymbol{r},\boldsymbol{R}) \quad (21)$$

where $\Delta_r = \frac{d^2}{d\boldsymbol{r}^2} + \frac{n-1}{\boldsymbol{r}}\frac{d}{d\boldsymbol{r}} - \frac{\ell(\ell+n-2)}{\boldsymbol{r}^2}$ and $\hat{\boldsymbol{L}}^2$ is the main orbital angular momentum operator. Then, separating the angular variable in Eq. (20) and defining the radial Laplacian operator in the 3-dimensional space and the ground state ($\ell = 0$), the Radial Schrodinger equation can be expressed as:

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right] + \frac{1}{8\mu^*}\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]^2 + \frac{q}{4\mu^*}\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]\cdot(\boldsymbol{B}\times\boldsymbol{r}) + \frac{q^2}{8\mu^*}(\boldsymbol{B}\times\boldsymbol{R})^2 - \frac{iq}{2\mu^*}(\boldsymbol{B}\times\boldsymbol{r})\cdot\nabla_r + V(\boldsymbol{r})\right)\varphi(\boldsymbol{r}.\boldsymbol{R}) = E(\mu^*)\varphi(\boldsymbol{r}.\boldsymbol{R}) \quad (22)$$

Within the Rytova-Keldysh potential (which shows the direct magnetoexciton orientation), the screened Coulomb potential (which shows the indirect magnetoexciton orientation), and assuming that in all center of mass frames, $P_R = 0$ (the momentum of the center of mass), we can obtain the state of the interaction and define a good approximation of the effect of temperature easier than solving the entire RSE with full potential interaction. So, the radial Schrödinger Eq. (22) in n dimensional space, at the finite temperature, and $\varepsilon_1 = \varepsilon_2$ can be shown as:

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right] + \frac{q^2}{8\mu^*}(\boldsymbol{B}\times\boldsymbol{r})^2 + \alpha_{RK}\boldsymbol{r} + \beta_{RK}\right)R(\boldsymbol{r}) = E(\mu^*)R(\boldsymbol{r}) \quad (23)$$

where

$$\alpha_{RK} = -\frac{q^2}{8\varepsilon_0\varepsilon r_0}H_0\left(\frac{1}{r_0}\right).\quad \beta_{RK} = -\frac{q^2}{8\varepsilon_0\varepsilon {r_0}^2}\left(H_0\left(\frac{D}{r_0}\right) - 0.367\right)$$

and

$$H_0(x) = 1.90\left(\frac{x}{3}\right) - 1.90\left(\frac{x}{3}\right)^3 + 0.68\left(\frac{x}{3}\right)^5 + \cdots$$

$$Y_0(x) = 0.36 + 0.60\left(\frac{x}{3}\right)^2 - 0.74\left(\frac{x}{3}\right)^4 + \cdots$$

Finally, the interlayer RK potential can be approximated by a harmonic type potential, as described in the next section.

5. Canonical variables transformation

To determine the eigenenergy and mass spectrum of the RSE (1), we applied the PUR. This technique is based on the QFT. Quantized fields can present as an assembly of harmonic quantum oscillators for the vacuum state. Most potentials have a different form than eigenfunctions in QM (i.e., differ from the Gaussian form), so the variables in the original RSE must be changed. The modified RSE should have solutions with the quantum oscillator manner at large intervals and distances, and after the commutation and transformation, a new structure of quantum specifics and numbers is obtained. This commutation is not canonical; instead, the transformation of variables leading to the Gaussian infinite-asymptote action in the d -dimensional axillary space is based on the PUR. Therefore, to use the QFT, we need to change the variables in equation RSE by inserting a new variable in the d-dimensional axillary space. Now, according to the high momentum asymptotic form of Gaussian type ($r \to \infty : r = q^{2\rho}$), Eq. (19) for $R(r)$ relative motion is:

$$R(r) \to R(r) = q^{2\rho\ell}\,\varphi(q^2) \quad (24)$$

$$\phi_0\left(\boldsymbol{r} - \frac{1}{q\boldsymbol{B}^2}(\boldsymbol{B}\times\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right]\right)exp\left(i\boldsymbol{R}\cdot(\left[-i\nabla_R - \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right] + \frac{q}{2}(\boldsymbol{B}\times\boldsymbol{r})\right)$$

and where ρ is a parameter to be determined, in the confining potential for an electron-hole system, this modification is performed using variational parameter ρ, and the magnetoexciton wave function becomes an oscillator one. The radial Laplacian operator in the d-dimensional axillary space, $d = 4\rho\ell + 2\rho + 2$ (ℓ is the angular momentum quantum number), can be defined using the radial Laplacian operator in the n-dimensional space [10,15].

$$\Delta_d = \frac{d^2}{dr^2} + \frac{n-1}{r}\frac{d}{dr} \rightarrow \Delta_q = \frac{d^2}{dq^2} + \frac{d-1}{q}\frac{d}{dq}$$

Hence, the wave function should have a Gaussian type solution for large distances, and we apply the PUR [10] variables from Eq. (9) to the Hamiltonian Eq. (10). After variables are expressed and changed into axillary space, the Hamiltonian is determined by:

$$\hat{H}_r \rightarrow \hat{H}_q = H_0 + \varepsilon_0(E) + :H_{Iq}: \tag{25}$$

where $\varepsilon_0(E)$ is the free oscillator Hamiltonian or the ground state vacuum energy, i.e., the minimum energy of the Hamiltonian. Now, based on PUR and the wick ordering method, we can define the creation ($\hat{a}^\dagger$) and the annihilation ($\hat{a}$) operator as follows:

$$[\hat{a},\hat{a}^\dagger] = 1 \quad , \quad \hat{a}\,|0\rangle = 0,$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\omega}}(m\omega\hat{q} - i\hat{p}) = \frac{1}{\sqrt{2m\omega}}\left(m\omega\hat{q} - \frac{\partial}{\partial\hat{q}}\right),$$

$$\hat{a} = \frac{1}{\sqrt{2m\omega}}(m\omega\hat{q} + i\hat{p}) = \frac{1}{\sqrt{2m\omega}}\left(m\omega\hat{q} + \frac{\partial}{\partial\hat{q}}\right),$$

$$\hat{q} = \frac{1}{\sqrt{2m\omega}}(\hat{a} + \hat{a}^\dagger), \quad \hat{p} = i\sqrt{\frac{m\omega}{2}}(\hat{a}^\dagger - \hat{a})$$

Then, the canonical variables in the quadratic models can be used to show increasing potential ($\hbar = c = 1$)[10]:

$$\hat{q}^{2n} = (-1)^n \frac{d^n}{dx^n} e^{-xq^2}|_{x=0} = (-1)^n \frac{d^n}{dx^n} \int \left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2\left(1+\frac{x}{\omega}\right)} :e^{-2i\sqrt{\pi}(q\eta)}:|_{x=0} =$$

$$\frac{(\frac{d}{2}+n-1)!}{(\frac{d}{2}-1)!}\omega^{-n} + n\omega^{1-n}\frac{(\frac{d}{2}+n-1)!}{(\frac{d}{2})!} :\hat{q}^2: + (-1)^n\omega^n \frac{d^n}{dx^n}\int \left(\frac{d\eta}{\sqrt{\pi}}\right)^d e^{-\eta^2(1+x)} :e_2{}^{-2i\sqrt{x\omega}(q\eta)}:|_{x=0}$$

where $e_2{}^x = e^x - 1 - x - 0.5x^2$, and according to the PUR conditions, the interaction Hamiltonian contains all non-square parts of the term :*: (a condition in Wick ordering). Hence, one can determine the Hamiltonian with $H_0 = \omega$ ($\hat{a}^+\hat{a}^-$), the energy of the pure oscillator, $:H_{Iq}:$, and the interaction Hamiltonian and the minimum energy of the coupled state $\varepsilon_0(E)$. Afterward, variables are expressed and changing into axillary space with $n = 1$.

$$\left[\hat{q}^2 \cong \frac{d}{2\omega} + :\hat{q}^2: \cong \frac{d}{2\omega} \quad \text{and} \quad \hat{p}_q^2 = \frac{d}{2}\omega + :\hat{p}^2: \cong \frac{d}{2}\omega\right]$$

$$\Rightarrow \quad \hat{H}_q = H_0 + \varepsilon_0(E) + :H_{Iq}: \tag{26}$$

Then, the energy of levels in the zeroth approximation of the PUR is obtained by minimizing the expectation value of Hamiltonian as follows:

$$\varepsilon_0(E) = min \int \Psi_0^* \hat{H}\, \Psi_0 dq = 0 \tag{27}$$

we can define the Schrödinger equation as follows:

$$\hat{H}\Psi = E(\mu)\Psi \Longrightarrow \left(\frac{\hat{p}_q^2}{2} + V(q)\right)\Psi = E(\mu)\Psi \tag{28}$$

and the free oscillator Hamiltonian as:

$$\varepsilon_0(E) = \frac{\hat{p}_q^2}{2} + \int \left(\frac{dk}{2\pi}\right)^d \left(\widetilde{V(k^2) - E}(k^2)\right) e^{-\frac{k^2}{4\omega}}$$

$$= \frac{\hat{p}_q^2}{2} + \int_0^\infty \frac{duu^{\frac{d}{2}-1}e^{-u}}{\left(\frac{d}{2}-1\right)!} W(u.E) = 0 \tag{29}$$

$$\varepsilon_0(E) = \frac{d\omega}{4} + 4\mu\rho^2 q^{4\rho-2}\left(V(q^{2\rho}) - E(\mu)\right) = 0 \tag{30}$$

In Eq. (30) one can define ρ using conditions $\frac{\partial E(\mu)}{\partial\rho} = 0$ for the Coulomb type potential $\rho \cong 1$.

Using conditions $\varepsilon_0(E) = 0$ and $\frac{\partial\varepsilon_0(E)}{\partial\omega} = 0$ from Eq. (30), one can define the pure angular velocity ω and the energy of the ground-coupled state in the oscillator explanation model [15].

6. The exciton bound state within the PUR method

6.1. The Rytova-Keldysh potential

In this study, we described the bound state of magnetoexciton within the Rytova-Keldysh potential when $r >> r_0$. In this case, RK potential diverges logarithmically at the origin and goes to the logarithmical dependence. Then, the interlayer RK potential can be approximated by a harmonic type potential as follows:

$$V_{RK}(r,T)_{r>>r_0} \rightarrow V(r,T) = \sigma r^2 - V_0 \tag{31}$$

where:

$$\sigma = -\frac{q^2}{16{r_0}^2 D\varepsilon_0\left(\frac{\varepsilon_1(T)+\varepsilon_2(T)}{2}\right)}\left(H_{-1}\left(\frac{D}{r_0}\right) - Y_{-1}\left(\frac{D}{r_0}\right)\right),$$

$$V_0 = \frac{q^2}{8{r_0}^2\varepsilon_0\left(\frac{\varepsilon_1(T)+\varepsilon_2(T)}{2}\right)}\left(H_0\left(\frac{D}{r_0}\right) - Y_0\left(\frac{D}{r_0}\right)\right)$$

and

$$H_{-\nu}(x) = (-1)^\nu H_\nu(x) + \sum_{j=0}^{\nu-1}\frac{(-1)^j}{\Gamma(j+1.5)\Gamma(j+1.5-\nu)}\left(\frac{x}{2}\right)^{2j+1-\nu}$$

$$Y_{-\nu}(x) = (-1)^\nu Y_\nu(x) = \frac{(-1)^\nu}{\pi}\left(\frac{x}{2}\right)^{-\nu}\sum_{j=0}^{\nu-1}\frac{\Gamma(\nu-k)}{\Gamma(k+1)}\left(\frac{x^2}{4}\right)^k + \frac{2}{\pi}J_\nu(x)ln\left(\frac{x}{2}\right) -$$

$$-\frac{(\frac{x}{2})^\nu}{\pi}\sum_{k=0}^{\infty}\Psi(\nu+k+1)\frac{\left(-\frac{x^2}{4}\right)^k}{\Gamma(k+1)\Gamma(\nu+k+1)}$$

and we know that at large distances, $r << r_0$, the RK potential becomes the Coulomb type potential:

$$V_{RK}(r,T)_{\boldsymbol{r}\ll\boldsymbol{r_0}} \to -\frac{q^2}{4\pi\varepsilon_0\left(\frac{\varepsilon_{1(T)}+\varepsilon_{2(T)}}{2}\right)}\frac{1}{\sqrt{r^2+D^2}} \quad (32)$$

Previous studies have proposed that the charged component electron and hole of magnetoexciton bound state in monolayer or multilayer materials at finite temperature can be utilized to determine new properties and characteristics of the bound state eigenenergy and mass spectrum, providing a plausible approximation to describe the features of 2D material systems [15,17].

6.2. Magnetoexciton bound state within the RK potential

The ground state eigenenergy ($\ell = 0$) of a magneto-exciton bound state in monolayer or multilayer 2D materials in a confining RK potential is presented in a theoretical framework based on quantum field theory. We start from Eq. (31) in $r >> r_0$, and then add Eq. (32) in $r << r_0$. Next, using Eqs. (23) and (26) and assuming $V_0 \approx 0$ and $\delta = \left(\frac{q^2}{8\mu^*}B^2 + \sigma\right)$, we have:

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2}+\frac{2}{\boldsymbol{r}}\frac{d}{d\boldsymbol{r}}\right]+\delta\boldsymbol{r}^2\right)R(\boldsymbol{r}) = E(\mu^*)R(\boldsymbol{r}) \quad (33)$$

Based on the projective unitary representation, the Hamiltonian of magnetoexciton bound state ($\hbar = c = 1$) for the principal quantum number $\ell = 0$ is defined as:

$$\frac{d\omega}{4}+4\mu^*\rho^2\delta\hat{q}^{8\rho-2}-4\mu^*\rho^2E(\mu^*)\hat{q}^{4\rho-2} = 0 \to$$
$$\frac{d\omega}{4}+4\mu^*\rho^2\delta\frac{(5\rho-1)!}{\rho!}\omega^{1-4\rho}-4\mu^*\rho^2E(\mu^*)\frac{(3\rho-1)!}{\rho!}\omega^{1-2\rho}=0 \quad (34)$$

where:

$$\omega^{\rho} = \left(16\rho^2\frac{(5\rho-1)!}{d\rho!}\left(\frac{q^2}{8}B^2 + \mu^*\sigma\right)\right)^{1/4} \quad (35)$$

and we can express the magnetoexciton eigenenergy as:

$$E_{\boldsymbol{RK-B}}(\mu^*) = \left(\frac{d\rho!\,(5\rho-1)!}{2\mu^*\rho^2}\left(\frac{q^2}{8\mu^*}B^2 + \sigma\right)\right)^{1/2} \quad (36)$$

Hence, one can define parameter ρ based on $\frac{\partial E(\mu^*)}{\partial\rho}=0$ and by using the equation of digamma function $\Psi(x)$ from Eq. (36), where $\Gamma(x) = (x\text{-}1)!$, by forming:

$$2.5\Psi(5\rho) - 1.5\Psi(3\rho) + 0.5\Psi(2\rho) - \rho^{-1} = 0 \quad (37)$$

Using the above equations, we have calculated and defined $\rho = 0.4913$.

6.3. Exciton bound state within the RK potential

We consider the exciton bound state from Eq. (31) in the RK potential as:

$$V(r,T) = -\frac{q^2}{16r_0{}^2D\varepsilon_0\left(\frac{\varepsilon_{1(T)}+\varepsilon_{2(T)}}{2}\right)}\left(H_{-1}\left(\frac{D}{r_0}\right)-Y_{-1}\left(\frac{D}{r_0}\right)\right) \cong \sigma\boldsymbol{r}^2 - V_0 \quad (38)$$

with orbital excited levels $\ell \neq 0$ without the magnetic field effect $\boldsymbol{B} = 0$ and $V_0 \approx 0$. The mass of the electron-hole bound state in the lowest oscillator frequency with a determination of the PUR method is presented. The eigenenergy of the relative Hamiltonian of the bound state [17,18] is:

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}\right]+\sigma\boldsymbol{r}^2\right)R(\boldsymbol{r}) = E_{RK}(\mu^*)R(\boldsymbol{r}) \to$$
$$\frac{(2+2\rho+4\rho\ell)\omega}{4}+4\mu^*\rho^2\hat{q}^{4\rho-2}\left(\sigma\hat{q}^{4\rho}-E_{RK}(\mu^*)\right)=0 \to \quad (39)$$
$$\frac{(2+2\rho+4\rho\ell)\omega}{4}+4\sigma\mu^*\rho^2\hat{q}^{8\rho-2}-4\mu^*\rho^2\hat{q}^{4\rho-2}E_{RK}(\mu^*)=0$$
$$\varepsilon_0(E) = \frac{(2+2\rho+4\rho\ell)\omega}{4}+4\sigma\mu^*\rho^2\frac{(2\rho\ell+5\rho-1)!}{(2\rho\ell+\rho)!}\omega^{1-4\rho}-4\mu^*\rho^2\frac{(2\rho\ell+3\rho-1)!}{(2\rho\ell+\rho)!}\omega^{1-2\rho}E_c(\mu^*)=0$$

According to conditions $\frac{\partial\varepsilon_0(E)}{\partial\omega}=0$ and $\varepsilon_0(E) = 0$, one can define the eigenenergy with the oscillator frequency relation:

$$\omega^{\rho} = \left(\frac{16\sigma\mu^*\rho^2}{3}\frac{(2\rho\ell+5\rho-1)!}{(2\rho\ell+\rho+1)!}\right)^{1/4}, \quad (40)$$
$$E_{RK} = \frac{(2\rho\ell+\rho+1)!}{8\rho^2\mu^*(2\rho\ell+3\rho-1)!}\omega^{2\rho}+\frac{\sigma(2\rho\ell+5\rho-1)!}{(2\rho\ell+3\rho-1)!}\frac{1}{\omega^{2\rho}} = \frac{2}{(2\rho\ell+3\rho-1)!}\left(\frac{\sigma(2\rho\ell+\rho+1)!(2\rho\ell+5\rho-1)!}{2\rho^2\mu^*}\right)^{1/4}$$

where ℓ is the principal quantum number and parameter $\rho \cong 0.5$ is determined by the equation $\frac{dE_c}{d\rho}=0$, and the binding energy of the hydrogen-like model is determined as $E_{bin}=\frac{1}{2n^2}\alpha_s{}^2\mu$. Hence, based on Eq. (41), one can determine that the masses of electrons and holes are equal $m_e{}^* = m_h{}^*$, $\mu = m_e{}^*/2$ in the binding energy of exciton in ground and excited states in mono elemental 2D nano-quantum materials, as follows:

$$E_{bin} = \frac{2}{(\ell+0{,}5)!}\left(\frac{2\sigma(\ell+0{,}5)!\,(\ell+1{,}5)!}{\mu^*}\right)^{1/4} - 4\mu^* \quad (41)$$

6.4. Exciton within the Coulomb potential

In this study, we presented the eigenenergy [16] of

an exciton state in mono elemental 2D nano-quantum materials within the Coulomb potential , and for indirect electron-hole bound, we set the relative coordinate $\sqrt{(r^2+D^2)}$. In the center of mass, we changed the variable to the cylindrical coordinate system $r = r(\zeta, \theta, z)$. $r = const.$ We considered that the Coulomb electrostatic potential in the cylindrical coordinate would depend on ζ and z, and not on θ due to axial symmetry. We changed the variables $\zeta = q^{2\rho}$, $R(\zeta, \theta, z) \rightarrow \Re(q^{2\rho})$, $\rho = 1$, $\boldsymbol{z} = D = const.$ for Coulomb type potentials and obtained the Hamiltonian of electron-hole interaction in the mono elemental 2D nano-quantum materials base on the PUR method. Therefore, the Schrödinger equation with $V_C(\boldsymbol{\zeta}, \boldsymbol{z}) = -\frac{q^2}{4\pi\varepsilon_r\varepsilon_0}\frac{1}{\sqrt{\zeta^2+z^2}} \cdot \sqrt{\boldsymbol{\zeta^2+z^2}} = \boldsymbol{r}$ can be expressed as:

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{1}{\zeta}\frac{d}{d\zeta}\left(\zeta\frac{d}{d\zeta}\right)+\frac{d^2}{dz^2}\right]-\frac{\alpha_C}{\varepsilon_r\zeta^2}\right)R(\boldsymbol{\zeta},\boldsymbol{z}) = E_C(\mu^*)R(\boldsymbol{\zeta},\boldsymbol{z}) \rightarrow \quad (42)$$

$$\left(-\frac{\hbar^2}{2\mu^*}\left[\frac{d^2}{d\zeta^2}+\frac{d}{\zeta d\zeta}-\frac{1+m^2}{\zeta^2}+\frac{d^2}{dz^2}\right]-\frac{\alpha_C}{\varepsilon_r\sqrt{\zeta^2+z^2}}\right)R(\boldsymbol{\zeta},\boldsymbol{z}) = E_C(\mu^*)R(\boldsymbol{\zeta},\boldsymbol{z})$$

Our excitonic system of 2D materials becomes a bound state separated by distance r. Then, similar to the previous Eqs. (33)-(37) in the theoretical framework of PUR [10] $V_c \cong -\frac{\boldsymbol{\alpha_C}}{\boldsymbol{\varepsilon_r r}}$, one can present Eq. (33) in the non-magnetic field interaction ($\hbar = c = 1$), $B = 0$, $r << r_0$, and $\rho \cong 1$, $d = 1+\rho+2\rho|m|$. In this paragraph, we consider the structure of nano-quantum materials within the Coulomb potential where $z = D = 0$ (i.e., the mono elemental 2D nano-quantum materials will serve as a nano-quantum dots parameter d) describes the dimension of the auxiliary space in the PUR method and one can determine as, and $m = 0, \pm1, \pm2, \cdots$ is the magnetic quantum number. By going to the new auxiliary $d = 2 + 2|m|$ dimension coordinate, we can present the modified Schrödinger equation as:

$$\left(-\frac{1}{2\mu^*}\left[\frac{d^2}{d\hat{q}^2}+\frac{1}{\hat{q}}\frac{d}{d\hat{q}}-\frac{1+2|m|}{\hat{q}^2}\right]-\frac{\alpha_C}{\varepsilon_r\sqrt{\hat{q}^2+\boldsymbol{z}^2}}\right)\Re(q) = E_C(\mu^*)\Re(\hat{q}) \quad (43)$$

with the magnetic quantum number $|m|$, which lets us define all bound state properties of an electron-hole, including the mass spectrum, eigenenergy, wave function, and spin-orbit interactions. Then, the ground state energy in the PUR method takes the form of Eq. (26).

$$\varepsilon_0(E) = \frac{d\omega}{4}+4\mu^*\hat{q}^2\left(-\frac{\alpha_C}{\varepsilon_r\hat{q}^2}-E_C(\mu^*)\right) = 0, \quad (44)$$

$$\varepsilon_0(E) = \frac{2+2|m|}{4}\omega-\frac{4\mu^*\alpha_C}{\varepsilon_r}-2(2+2|m|)\mu^*\omega^{-1}E_C(\mu^*) = 0$$

Under conditions $\varepsilon_0(E) = 0$, $\frac{\partial\varepsilon_0(E)}{\partial\omega} = 0$, and $\mu^* = \frac{m_e^*m_h^*}{2m_e^*+\mu_h^*}$ the parameter represents the boundary system's component mass in mono elemental nanolayers (the reduced mass of the system). The eigenenergy of the relative Hamiltonian is defined as:

$$E_C(\mu^*) = \frac{1}{8\mu^*}\omega^2-\frac{\alpha_C}{\varepsilon_r}\frac{1}{|m|+1}\omega \quad (45)$$

where $\omega = \frac{4\alpha_s\mu^*}{(|m|+1)\varepsilon_r}$; hence, the eigenenergy of the electron-hole bound state is:

$$E_C(\mu^*) = -2\mu^*\left(\frac{\alpha_C}{(|m|+1)\varepsilon_r}\right)^2 \quad (46)$$

Then, the binding energy of exciton in the mono elemental 2D nano-quantum materials is determined by:

$$E_{bin} = -2\mu^*\left(\left(\frac{\alpha_C}{(|m|+1)\varepsilon_r}\right)^2+2\right) \quad (47)$$

6.5. Exciton within QFT approaches

In this section, we describe how massless quasiparticles (holes) suddenly acquire mass in the relativistic limit of interactions. In QFT, the bound state of an electron-hole as an exciton system can be realized:

1- if $M \neq m_e + m_h$ and $M < \infty$, then a bound state with a mass M arises.

2- if $M = m_e + m_h$, tthen the interaction is so weak that the bound state can not arise, and the scalar particle exists as two independent states. Therefore, the mass spectrum and energy of a free exciton in mono elemental or non-mono elemental nanolayers can be defined very accurately in the context of RQM and QFT. As the relativistic behaviors of an exciton, the electron-hole bound states are very important in the field of nanomaterials and nano quantum dots within a strong Coulomb type interaction which can be expressed as $V(r) = -\alpha_s r^{-1}$. So, the theoretical description is reduced to determine the relativistic modification and regulate the interaction based on QFT theories. This idea defines the relativistic corrections using Feynman path integral, i.e., determines the interaction potential of the bound state and the relativistic behavior of mass. This idea is presented in more detail in section 2. To use the proposed formulas to describe the exciton bound state, eigenenergy, and mass spectrum based on QFT and

$V(r) = \alpha_s r^{-1}$, we assumed the electron and hole mass interact solely within the strong Coulomb potential, i.e., we ignored the concept of effective mass and assumed the system was completely relativistic with a high energy interaction due to the large amount of photon energy. The radial relativistic Schrödinger Eq. (11) $\hat{H}R = \varepsilon R$ can be presented in the modified form Eqs. (3), (4), (8) and (9) with $|\hat{\boldsymbol{p}}_{\boldsymbol{e}}^{\boldsymbol{2}}| = |\hat{\boldsymbol{p}}_{\boldsymbol{e}}^{\boldsymbol{2}}| = |\hat{\boldsymbol{p}}_{\boldsymbol{r}}^{\boldsymbol{2}}|$ in the projective unitary method. This method is used to determine the bound states mass spectrum (M) and eigenenergy (ε). The relative Hamiltonian of the electron-hole bound state with a strong $V(r)$ potential presented in Eq. (10) is modified to express the relativistic corrections (using Feynman path integral) as follows:

$$\hat{H}\Psi = \varepsilon\Psi \Rightarrow \left[\frac{\hbar^2}{2}\left(\mu_e + \frac{m_e^2+\hat{p}_r^2}{\mu_e}\right) + \frac{\hbar^2}{2}\left(\mu_h + \frac{m_h^2+\hat{p}_r^2}{\mu_h}\right) + V(\boldsymbol{r})\right]\Psi = M\Psi \Rightarrow$$

$$\left[\frac{\hbar^2}{2\mu}\hat{p}_r^2 + V(\boldsymbol{r})\right]\Psi = \left[M - \frac{\mu_e+\mu_h}{2} - \frac{m_e^2\mu_h+m_h^2\mu_e}{2\mu_e\mu_h}\right]\Psi \quad (48)$$

$$\frac{1}{\mu} = \frac{1}{\mu_e} + \frac{1}{\mu_h} = \frac{1}{\left(m_e^2 - 2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2}} + \frac{1}{\left(-2\mu^2\frac{dE(\mu)}{d\mu}\right)^{1/2}} \quad (49)$$

where μ_e and μ_h are the constituent mass of components (electron and hole) in the bounding system and μ is the reduced mass of electron-hole bound state that is determined and presented in section 2. Next, we determined the eigenenergy and mass spectrum of the electron-hole bound state. From Eq. (11) and $\left[\hat{q}^2 = \frac{d}{2\omega}, \hat{p}_q^2 = \frac{d}{2}\omega\right]$, $\rho = 1$, $d = 4 + 4\ell$ one can define the eigenenergy of the ground using $\varepsilon_0(E) = 0$ and $\frac{\partial\varepsilon_0(E)}{\partial\omega} = 0$ as follows:

$$\varepsilon_0(E) = (\ell+1)\omega - 4\mu\alpha_s - \frac{8(\ell+1)\mu E_c(\mu)}{\omega} = 0 \rightarrow \quad (50)$$

$$E_c = -\frac{1}{2}\left(\frac{\alpha_s}{(\ell+1)}\right)^2\mu \rightarrow E_c = -\frac{1}{2}\beta\left[\frac{\left((m_e^2+\mu^2\beta)\mu^2\beta\right)^{1/2}}{(m_e^2+\mu^2\beta)^{1/2} + (\mu^2\beta)^{1/2}}\right]$$

where $\frac{dE_c}{d\mu} = -\frac{1}{2}\left(\frac{\alpha_s}{(\ell+1)}\right)^2 = -\frac{1}{2}\beta$ and the oscillator frequency relation is:

$$\frac{dE_c}{d\mu} = -\frac{1}{2}\left(\frac{\alpha_s}{(\ell+1)}\right)^2 = -\frac{1}{2}\beta$$

Then, the mass spectrum of an exciton is determined using Eq. (2):

$$M = (m_e^2 + \mu^2\beta)^{1/2} + (\mu^2\beta)^{1/2} - \beta\mu \quad (51)$$

where the constituent mass of components is defined as

$$\mu_e = (m_e^2 + \mu^2\beta)^{1/2}, \quad \mu_h = (\mu^2\beta)^{1/2}. \quad (52)$$

Hence, one can easily determine the parameter $\mu = \frac{\mu_e\mu_h}{\mu_e+\mu_h}$ by solving the Eq. (53).

$$(A^2-\beta^2)\,\mu^4 + (2AB-4\beta m_e^2)\,\mu^2 + B^2 = 0 \quad (53)$$

with $A = \beta^2 - 2\beta$ and $B = m_e^2\beta - m_e^2$.

The parameter μ and μ^* are completely different and distinct concepts. Next, we determine the parameters of the exciton, composed of an electron and hole under the strong Coulomb interaction in mono elemental nanolayers. The following limits on the cluster's rest mass are currently established as m_e = 051099895 MeV, m_h = 0, with a weak and strong Coulomb constant interaction range of $0.007 \leq \alpha_s \leq 0.21$, in the ground and excited states and without spins-orbital interactions. The relative mass spectrum results of the electron mass $\sigma_\ell = \frac{M_{nonrel}}{m_e}, \sigma_{rel-\ell} = \frac{M_{rel}}{m_e}$ of exciton are presented in Fig. 2.

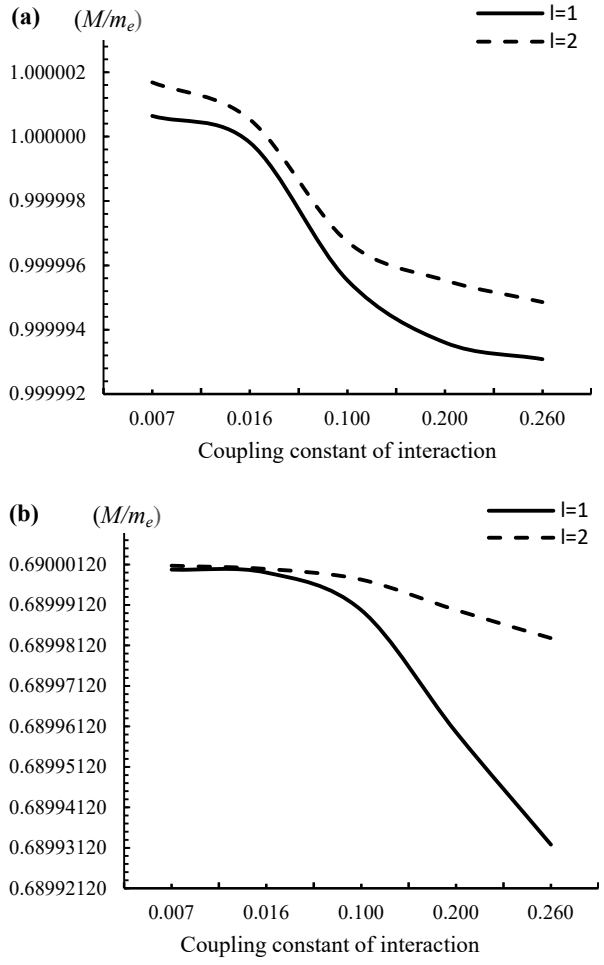

Fig. 2. The theoretical value of free exciton bound state in Silicene (mono-elemental Si Fs) with relativistic correction (a) and without (b), for the ground ($\ell = 0$) and excited states ($\ell = 1$).

The different properties and characteristics of bound states in mono elemental 2D Xenes nanolayer materials have been previously determined and defined [19,20]. The theoretical calculation with the average coupling $\langle\alpha_s\rangle = 0.1166$ relation of relativistic to non-relativistic mass coefficient $\langle\frac{\sigma_{rel-\ell}}{\sigma_\ell}\rangle$ for the ground state $\ell = 0$ and excited state $\ell = 1$ were determined as 1.44932 and 1.44928, respectively. The benefit of this correction and interacting effects of the electron-hole based on QFT can be shown theoretically by the relativistic effect of the coupling (which mixes states with different multiplicities, e.g., singlet-triplet spin transition, photon, polariton, etc.), correlations, and effects. Studies on electron-hole bound state interactions have intensified with the construction and formation of quantum systems confined in spatial dimensions known as artificial-exotic atoms, super atoms, and magnetoexciton in the presence of a magnetic field. Due to their physical properties, there has been a great deal of recent interest and research in these exotic systems for use in quantum technologies, quantum computers, solar cells, quantum dot lasers, electrically tunable spin qubits, electrical manipulation of individual spins, and transistors, etc. [23-25]. "In 1994, Wagner *et al.* predicted a transition for the ground state energy from the spin-singlet to the spin-triplet state as a function of the magnetic field [26, pp. 1953]". Since then, the numerical diagonalization of the Hamiltonian matrix, variational approach, Hartree-Fock method, and other methods and techniques have been used to determine and calculate the energy levels of nano quantum materials.

In this study, the PUR method was presented to determine the eigenenergy levels of MEM based on describing the relationship between relativistic corrections to the effective mass of particles. According to the results, we can define and determine spin eigenenergy by determining the weak or strong electron-hole interaction in MEM. The benefit of these corrections and correlation effects of interacting electrons confined in a MEM can be shown in theoretical and experimental ways. Due to the MF effect on spin transitions and adaptation, we conclude that the quantum environment of MEM has good potential to be a new candidate for future quantum processors and quantum technologies. Hence, one of the major advantages of the use of the relativistic correction to the mass in the total Hamiltonian is the possibility to determine and consistently yield more accurate results of the transition characteristic in MEM. Since we do not investigate the effects of spin interactions in this article, it is worth mentioning how the relativistic correction of mass can affect the results of the total eigenenergy of a MEM [26]. Nano-quantum materials show potential as new candidates for future quantum processors and quantum technologies because of the magnetic field effect on the bound state, spin transitions, and adaptation. Hence, one of the major advantages of the use of the relativistic correction to the mass in the total Hamiltonian is the possibility to determine and consistently yield more accurate results of the properties and characteristics in high-tech materials.

7. Conclusion

A new approach for predicting the mass spectrum of extraordinary electron-hole coupled states in mono and non-mono elemental nanolayers, based totally on the relativistic-quantum model and the quanto-relativistic behavior of the electron-hole coupled system within a strong electromagnetic and RK potential has been presented and investigated. The most important problem of technology and investigations in mono elemental nanolayers is the generation principles of the ground states and energy levels of the electron-hole bound states. In summary, the following situation can be realized:

i) If $\delta \leq M < \infty$ and $M \neq m_1 + m_2$, $0 > \mu_i \geq \vartheta$, then a magnetoexciton with a mass M arises. δ and ϑ are dimensionless parameters that can be described by the coupling constant value and the mass of the electron (hole) in the binding system at the zero velocity, where M is the mass of coupled electron-hole and μ_i is the constituent mass of the electron (hole).

ii) If $M = m_1 + m_2$, then the interaction is so weak that the electron-hole coupled state cannot arise and the electron and hole exist as different free particles with definite energy in mono elemental nanolayers.

Based on these situations, we successfully defined the eigenenergy, the constituent mass, the free angular velocity, and the reduced mass of magnetoexciton in the mono elemental nanolayers. The relativistic to non-relativistic mass coefficients were theoretically determined as 1.44932 for the ground state and 1.44928 for the first excited state. Relativistic quantum mechanics offers a unique opportunity to investigate

the dynamics of magnetoexciton-related systems. The features of exotic atoms based on the relativistic behavior of the interaction are excellent tools to extract useful information on magnetoexcitons in the mono elemental nanolayers. Our understanding of relativistic quantum mechanics and QFT provides a good method for investigating quasi-atoms containing a hole and an electron. Most of the studied exotic linked systems are made up of a hole coupled to an electron because the attracting force of the clusters (the hole and the electron) creates related states, becoming more stable systems. Systematic studies of magnetoexciton energy levels have extracted considerable detail on magnetoexciton interactions. In this theoretical work, the eigenenergy of magnetoexciton in mono elemental nanolayers was determined based on relativistic corrections to the particles of the hole and the electron. Moreover, we defined that the constituent masses of the hole and the electron are different from the hole and electron in a resting state and close to the effective masses. Both mass spectrum and constituent masses were theoretically defined and presented. Also, the eigenenergy of electron-hole coupled in the mono elemental nanolayers was estimated with the Coulomb potential within the magnetic field, based on the projective unitary representation of the symplectic group, QFT ideas, and the normal order method. We defined the free angular velocity value of creating a coupling state and defined the mass of the bonding electron-hole system in mono elemental nanolayers with the minimum value in the relativistic limit. We denoted that the constituent masses are different from the effective masses of an electron and a hole. This computational achievement can be very useful in future research on monolayers, bilayers, and mono elemental nanolayers. Since results from new experiments on mono elemental nanolayers continue to be obtained, future in-depth investigation and determination of magnetoexciton characteristics are needed. We aim to investigate this type of prediction on magnetoexciton-polariton and multi-exciton systems trapped in mono and non-mono elemental nanolayers in future works.

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