TRƯỜNG ĐẠI HỌC SƯ PHẠM TP HỒ CHÍ MINH
TẠP CHÍ KHOA HỌC
KHOA HỌC TỰ NHIÊN VÀ CÔNG NGHỆ
Tập 14, Số 9 (2017): 43-50

HO CHI MINH CITY UNIVERSITY OF EDUCATION
JOURNAL OF SCIENCE
NATURAL SCIENCES AND TECHNOLOGY
Vol. 14, No. 9 (2017): 43-50

ISSN: 1859-3100

Email: tapchikhoahoc@hcmue.edu.vn; Website: http://tckh.hcmue.edu.vn

BINDING ENERGY OF EXCITON IN MONOLAYER SEMICONDUCTOR WS_2 WITH YUKAWA-LIKE SCREENING POTENTIAL

Le Dai Nam [1], Hoang Do Ngoc Tram[2*]

[1] Ton Duc Thang University

[2] Ho Chi Minh City University of Education

Received date: 17/7/2017; Revised date: 30/7/2017 Accepted date: 23/9/2017

ABSTRACT

The Yukawa-like screening potential is suggested to describe the effect of environment on the binding energy of an exciton in the monolayer semiconductor WS_2. The FK Operator Method combined with the Levi-Civita transformation is used to retrieve energies for the states of n= 1, 2, 3 which agree with experimental data. Experimental values of the parameters in the screening potential expression are also obtained for further use in the case of presence of external field.

Keywords: monolayer semiconductor, exciton, energy, FK operator method, Schrödinger equation, screening potential.

TÓM TẮT

Năng lượng liên kết của exciton trong bán dẫn đơn lớp WS_2 với thế màn chắn dạng tựa Yukawa

Thế màn chắn dạng tựa Yukawa được đưa ra để mô tả ảnh hưởng của môi trường lên năng lượng của exciton trong bán dẫn đơn lớp WS_2. Phương pháp toán tử FK kết hợp với phép biến đổi Levi-Civita được sử dụng. Kết quả thu được năng lượng cho các trạng thái n= 1, 2, 3 phù hợp với số liệu thực nghiệm. Các giá trị thực nghiệm của các tham số trong biểu thức thế chắn tựa Yukawa cũng được tính toán để làm cơ sở phát triển cho trường hợp có trường ngoài.

Từ khóa: bán dẫn đơn lớp, exciton, năng lượng, phương pháp toán tử FK, phương trình Schrödinger, thế màn chắn.

1. Introduction

Thanks to experimental achievements in growing two-dimensional semiconductor systems such as monolayer transition metal dichacogenides (TMDs), exciton in two-dimensional semiconductor becomes an interesting researched object because the main optical transitions in this semiconductor system is forming excitons. These researches provide information for explaining physics nature as well as for applying in optical and electronic devices of TMDs [1-2].

In the previous works [3-5], the FK Operator Method (FK-OM) [6, 7] was applied to finding exact solutions (energies and wavefunctions) for the Schrödinger equation of a two-dimensional exciton in a magnetic field, in which exciton is considered an isolated

[*] Email: *ngoctramhd@gmail.com*

system. The Levi-Civita transformation is used to transform the problem under investigation into the one of an anharmonic oscillator. The energies (and wavefunctions) for any states corresponding to arbitrary intensity of magnetic field with the precision up to 20 decimal places were obtained. In addition, highly accurate asymptotic solutions for the ground state and some excited states were also given.

However, recent works show that effect of surrounding environment on energy spectrum cannot be neglected when explaining experimental data. In the work [8], the authors showed that theoretical calculations for the ground state energy of exciton in monolayer semiconductor WS_2 when neglecting the environmental effect is 1 eV, while corresponding experimental result is 0.32 eV. This difference is regulated by taken into account of screening effect of surrounding electrons on Coulomb interaction between the hole and the electron in exciton which described by the variation of dielectric constant. In addition, the author used the formula of screening Coulomb potential suggested by Keldysh [9] for explaining obtained experimental result. Thus, experimental result can be explained by considering environmental effect via screening Coulomb potential when calculating theoretically.

For the goal of developing the FK-OM for obtaining exact solutions which appropriates with experimental results, considering screening effect is essential. However, the formula of Keldysh screening potential is too complicated to apply the FK-OM to the problem and develop for more complex physics system. In the work [10], the FK-OM was used to calculate energy of two-dimensional exciton with taken into account of environment effect under the form of Yukawa screening potential [11]. However, only theoretical results were given without comparing with experimental data. For developing previous researches, in this work, we modify the Yukawa screening potential in order to appropriate with the curve of Keldysh screening potential and still keep the convenient form for calculation. Then, the FK-OM combined with the Levi-Civita transformation [7] is applied to find energy of two-dimensional exciton under screening effect and retrieve screening parameter by comparing the obtained results with experimental data.

The paper is presented in following structure: first is an introduction; then the Yukawa-like potential modified to appropriate with the Keldysh potential is given; after that, the FK-OM combined with the Levi-Civita transformation is applied to two-dimensional exciton in screening potential; results and discussion is also presented; finally is conclusion.

2. The Yukawa-like screening potential

In the work [9], Keldysh suggests the screening potential under the form:

$$V_K = -\frac{\pi e^2}{2r_0}\left[H_0\left(\frac{r}{r_0}\right) - Y_0\left(\frac{r}{r_0}\right)\right], \qquad (1)$$

in which $H_0(x)$ and $Y_0(x)$ are Struve and second kind Bessel functions, respectively; r_0 is screening distance characterizing for the semiconductor, values of r_0 are determined by fitting theoretical results and experimental data. The Keldysh screening potential is used in theoretical calculation to explain experimental energy of a two-dimensional exciton in monolayer semiconductor WS_2 [8].

In the work [10], the FK-OM is applied to the problem of two-dimensional exciton in a magnetic field with the presence of the well-known Yukawa screening potential:

$$V_Y = -\frac{\exp(-\lambda r)}{r}, \tag{2}$$

in which λ is screening potential characterizing for environmental effect.

The Yukawa screening potential has a much simpler form than the Keldysh potential form, so it is convenient for using in calculating. However, this potential is not exact enough to explain experimental results. From the expression of the Yukawa screening potential and the asymptotic behaviors of Keldysh screening potential, we suggest the Yukawa-like screening potential as follow

$$V = -\frac{\alpha \exp(-\lambda r) + \beta}{r}, \tag{3}$$

in which α, β and λ are parameters for regulating the curve of potential. In the work [8], the screening distance value in (1) is $r_0 = 75\,\mathring{A}$. Fitting the functions (1) and (3) by using the least square method and fixed the curves at two points $r_1 = 0.5a_o^*$ and $r_2 = 9.5a_o^*$ which is the boundary of the effective zone of screening potential [8], in which a_o^* is effective Borh radius of exciton in two-dimensional semiconductor. Corresponding to the screening distance $r_0 = 75\,\mathring{A}$ in formula (1), we obtain the parameters in the Yukawa-like screening potential in the formula (3) are $\alpha = 0.636509$, $\beta = 0.670462$ and $\lambda = 0.174423$. At that time, the relative error between the two curves is below 6.5% (see Fig. 1). However, these values are just for illustrating the ability of replacement the Keldysh potential by the Yukawa-like potential. Experimental values of these parameters will be determined in the next part when we fitting the theoretical results with experimental data [8].

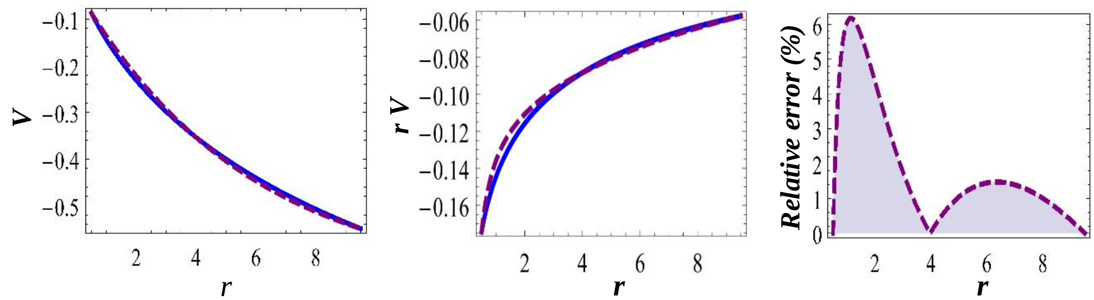

Fig. 1. *Comparing Keldysh screening potential V_K (solid curves) and the Yukawa-like screening potential fitted using least square (dashed curves), the two curves have similar shape and the relative error is below 6.5%.*

3. The FK-OM for two- dimensional exciton with screening potential

In the previous works [3-5], the Schrödinger equation for a two-dimensional exciton in a magnetic field in the space (x, y) is transformed into the Schrödinger equation for a two-dimensional anharmonic oscillator in the space (u,v) which is convenient for algebraic calculation by using the Levi-Civita transformation: $x = u^2 - v^2, \quad y = 2uv$. Similarly, in this work, the Schrödinger equation for a two-dimensional exciton with the presence of the Yukawa-like screening potential is rewritten in the two-dimensional space (u,v) as follows:

$$\tilde{H}\ \Psi(u,v) = 0\ , \tag{4}$$

$$\tilde{H} = -\frac{1}{8}\left(\frac{\partial^2}{\partial u^2} + \frac{\partial^2}{\partial v^2}\right) - E(u^2+v^2) + \alpha \exp\left[-\lambda\left(u^2+v^2\right)\right] + \beta. \tag{5}$$

Here, the notations and units are the same to the work [3].

For finding the solutions of equation (4)-(5), we use the FK-OM with the process described in the work [3]. There is only one difference that the term of Coulomb interaction in [3] is replaced by the term of the Yukawa-like screening potential

$$\hat{S}_{Yuk} = \alpha \exp\left[-\lambda\left(u^2+v^2\right)\right] + \beta \tag{6}$$

which can be easily represented in the algebraic form for applying the FK-OM [4].

Here, we remind the main idea of the FK-OM which is similar to the perturbation theory: the Hamiltonian is divided into two parts, in which the main part is an operator having exact analytical solutions; these eigenfunctions become the basic set of wavefunctions. When applying the FK-OM for problems of two-dimensional atomic system, thanks to the Levi-Civita transformation, the Schrödinger equation for two-dimensional atomic system in the space (x, y) is rewritten under the form of the Schrödinger equation of a two-dimensional anharmonic oscillator in the space (u,v) [3, 7].

Therefore, the basic set is chosen as the set of eigenfunctions of two-dimensional harmonic oscillator in the space (u,v) with the frequency of ω being considered a free parameter. The total Hamiltonian of the problem does not depend on this parameter while the two separated parts of Hamiltonian depend on it. Thus, we can regulate the value of ω in order that the main part becomes much larger than the perturbative part to increase the convergent rate [3].

The zeroth order approximate energy corresponding to the basic set of two-dimensional harmonic oscillator wavefunctions $\left|n(m)\right\rangle$ as follow:

$$E_{nm}^{(0)} = \frac{\omega^2}{2} + \frac{2\omega\beta}{2n+1} + \frac{2\alpha\omega}{(2n+1)(\mu+1)^{2n+1}} F_0\left(n,m,\mu^2\right), \tag{7}$$

with $\mu = \dfrac{\lambda}{2\omega}$; $F_0(n,m,x)$ is hypergeometric function defined as follow:

$$F_j(n,m,x) = {}_2F_1(m-n,-m-n;\, j+1;\, x) = \sum_{k=0}^{n-|m|} \frac{j!(n-m)!(n+m)!}{k!(k+j)!(n-m-k)!(n+m-k)!} x^k .$$

From the condition that the exact solutions of the problem do not depend on the value of the free parameter ω, we can rewritten the expression describing this condition at the zeroth-order approximation as follow

$$\frac{\partial E_{nm}^{(0)}}{\partial \omega} = 0 \tag{8}$$

for determining value of ω.

Higher order approximate solutions can be obtained by using the perturbation theory scheme via the two following equations [3]:

$$E_n^{(s)} = \frac{H_{nn}^R + \sum\limits_{k=|m|, k\neq n}^{n+s} C_k^{(s)} H_{nk}^R}{R_{nn} + \sum\limits_{k=|m|, k\neq n}^{n+s} C_k^{(s)} R_{nk}} . \tag{9}$$

$$\sum_{k=|m|,\, k\neq n,\, k\neq j}^{n+s} \left(H_{jk}^R - E^{(s-1)}\right) C_k^{(s)} = R_{nj} E^{(s-1)} - H_{nj}^R , \tag{10}$$

in which $j = |m|,\ |m|+1, \ldots,\ n-1,\ n+1, \ldots,\ n+s$ and non-zero matrix elements of Hamiltonian are:

$$\tilde{H}_{nn}^R = \left(\frac{\omega}{4} + \frac{m\gamma}{4\omega}\right)(2n+1) + \frac{\gamma^2}{32\omega^3}(2n+1)(5n^2+5n+3-3m^2) + \alpha S_{nn} ,$$

$$\tilde{H}_{n,n+1}^R = \left(-\frac{\omega}{4} + \frac{m\gamma}{4\omega} + \frac{3\gamma^2}{64\omega^3}(5n^2+10n+6-m^2)\right)\sqrt{(n+1)^2 - m^2} + \alpha S_{n,n+1} ,$$

$$\tilde{H}^R_{n,n+2} = \frac{3\gamma^2}{64\omega^3}(2n+3)\sqrt{(n+1)^2-m^2}\sqrt{(n+2)^2-m^2} + \alpha S_{n,n+2}, \qquad (11)$$

$$\tilde{H}^R_{n,n+3} = \frac{\gamma^2}{64\omega^3}\sqrt{(n+1)^2-m^2}\sqrt{(n+2)^2-m^2}\sqrt{(n+3)^2-m^2} + \alpha S_{n,n+3},$$

$$\tilde{H}^R_{n,n+s} = \alpha S_{n,n+s}, \quad (s \geq 4)\ ,$$

with $S_{n,n+s} = \frac{1}{s!}\sqrt{\frac{(n+s-m)!(n+s+m)!}{(n-m)!(n+m)!}}\frac{(-\mu)^s}{(1+\mu)^{2n+s+1}}F_s(n,m,\mu^2), \qquad (12)$

and $R_{nn} = \langle n(m)|\tilde{R}|n(m)\rangle = \frac{2n+1}{2\omega}, R_{n,n+1} = \langle n(m)|\tilde{R}|n+1(m)\rangle = -\frac{1}{2\omega}\sqrt{(n+1)^2-m^2}\ . \qquad (13)$

By using symmetric property $\tilde{H}^R_{nk} = \tilde{H}^R_{kn}$, we can find out other non-zero matrix elements.

4. Results and discussion

By using the scheme (9)-(10) and the matrix elements (11)-(13), we program on the language of FORTRAN 77 to build a code for calculating exact numerical solution of the problem. This program allows calculate energy and wavefunction for any states with the precision of up to 20 decimal places. The parameters in the expression of the Yukawa-like screening potential (3) are chosen in order that obtained energies fitted with experimental data in [8]. The results show that with $\alpha = 0.754095$, $\beta = 0.680177$ and $\lambda = 0.163479$, theoretical results agree with experimental data. In the Table 1, we show the values of theoretically calculated energies and experimental ones. Here, the experiment energies have the precision of only two decimal places with a measurement error, so the two results are considered agreed when the theoretical values is in the range of significant values of experimental data. In addition, notice that the screening effect decreases its influence for high excited states; we can see that the theoretical and experimental values agree well in the 1s and 2s state. The small difference between theoretical and experimental values can be explain that the sample in experimental was supported by SiO_2 while theoretically calculated binding energies for ideal, isolated samples ("floating in vacuum").

Although having simple form, the Yukawa-like screening potential allows describing environmental effect on binding energy of exciton in monolayer WS_2. The process of the FK-OM for the problem under investigation still remains the same as in the work [3]; the calculation is applied to concrete system of WS_2 but can be applied for similar monolayer semiconductor. Therefore, the FK-OM can be applied to investigate various similar systems and can be developed for more complex two dimensional atomic systems such as considering the presence of external field or applying to charged exciton.

Table 1. *Comparing experimental binding energies of exciton in monolayer semiconductor WS_2 [8] and theoretical ones by using the FK-OM with taken into account of Yukawa-like screening potential. These results agree with each other*

	Theory			Experiment
	$E_{binding}$ $\left(2Ry^{*}=0.16Ry\right)$	$E_{binding}$ $\left(eV\right)$	$E_n = E_{gap} - E_{binding}$ $\left(E_{gap} = 2.41eV\right)$	E_n $\left(eV\right)$
1s	0.073998	0.322039296	**2.088**	2.088 ± 0.01
2s	0.032911	0.143228672	**2.266**	2.25 ± 0.01
3s	0.018011	0.078383872	**2.331**	2.308 ± 0.01
4s	0.011313	0.049234176	**2.360**	2.34 ± 0.02
5s	0.075167	0.032712678	**2.375**	2.368 ± 0.02

5. Conclusion:

In this work, effect of environment can be described by the simple expression of the Yukawa-like screening potential which allows applying the FK-OM to find the binding energy of a two-dimensional exciton in monolayer WS_2. Although the problem under investigation is more complex and more reality than previous problems without considering screening effect, the calculation by the FK-OM still remains the same process. The obtained energies coincide with experimental data. This result is also a foundation for developing the FK-OM for more complex two dimensional atomic systems with taken into account of screening effect.

Acknowledgment: *This research is funded by Vietnam National Foundation for Science and Technology Development (NAFOSTED) under grant number 103.01-2016.90 and by HCMC University of Education under grant number CS2016.19.13.*

REFERENCES

[1] Mak K. F. and Shan J., "Photonics and optoelectrics of 2D semiconductor transition metal dichacogenides," *Nature Photonics* **10**, pp. 216-226, 2016.

[2] Hao K. et al., "Direct measurement of exciton valley coherence in monolayer WSe_2," *Nature Phys.* **12**, pp. 1-7, 2016.

[3] Hoang-Do Ngoc-Tram, Pham Dang-Lan and Le Van-Hoang, "Exact numerical solutions of the Schrödinger equation for a two-dimensional exciton in a homogeneous magnetic field of arbitrary strength," *Physica B* **423**, pp. 31-37, 2013.

[4] Hoang-Do Ngoc-Tram, Hoang Van-Hung and Le Van-Hoang, *Analytical solutions of the Schrödinger equation for a two-dimensional exciton in magnetic field of arbitrary strength*, J. Math. Phys. **54**, 052105, 2013.

[5] Hoang D. Ngoc-Tram, Nguyen P. Duy-Anh, Hoang Van-Hung and Le Van-Hoang, "Highly accurate analytical energy of a two-dimensional exciton in a constant magnetic field," *Physica B* **495**, pp. 16-20, 2016.

[6] Feranchuk I. D. and Komaro L. I., "The operator method of the approximate solution of the Schrödinger equation," *Physics Letters A* **88**, 5, pp. 211-214, 1982.

[7] Feranchuk I. D., Ivanov A., Le Van-Hoang and Ulyanhenkov A., *Non Perturbative Description of Quantum Systems*, Springer – Switzerland.

[8] Chernikov A., Berkelbach T. C., Hill H. M. et al, "Exciton binding energy and nonhydrogenic Rydberg series in monolayer WS_2", *Phys. Rev. Lett.* **113**, pp. 076802-5, 2014.

[9] Keldysh L. V., "Coulomb interaction in thin semiconductor and semimetal films", *JETP Lett.* **29**, pp. 658-661, 1979.

[10] Le Van Hoang, Le Tran The Duy, Hoang Do Ngoc Tram et al., "Exact solution of two-dimensional screened donor states in a magnetic field," *Comm. Phys.*, Suppl. **2004**, pp. 58-63, 2004.

[11] Soylu A. and Boztosun I., "Asymptotic iteration method solution of the energy spectrum of two-dimensional screened donor in a magnetic field", *Physica E* **40**, 3, pp. 443-448, 2008.