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Solutions of Two-dimensional Schrodinger Equation in Symmetries of Extended Quantum Mechanics for the Modified Pseudoharmonic Potential: an Application to Some Diatomic Molecules

Abdelmadjid Maireche[*]

Laboratory of Physics and Material Chemistry, Physics Department, Sciences Faculty, University of M'sila, M'sila Algeria

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The search for solutions of Schrödinger equation (SE) with physically motivated potential models has led to the discovery of new physical and chemical phenomena. For example, the pseudoharmonic oscillator potential (PHOP) has a very interesting history: it is often used to compute bound-state normalizations and energy levels of some diatomic molecules. This research has been divided into two parts. Firstly, we have converted the mechanical properties related to the force constant, the equilibrium bond length, the orthonormalized wave function and the energy eigenvalues to the corresponding atomic properties, which include the dissociation energy and equilibrium intermolecular separation for the purpose of applying to the homonuclear diatomic molecules, such as O_2, N_2 and H_2, and heteronuclear diatomic molecules, such as CH and ScH, under 2D-PHOP. Secondly, we have investigated some aspects of the modified 2D-PHOP (2D-MPHOP) in noncommutative 2D real space-phase (NC: 2D-RSP) through the generalized Bopp's shift method in the framework of parameters due to (space-phase) noncommutativity ($\theta,\bar{\theta}$) by means of the solution of the 2D-deformed SE (2D-DSE). We have reconstructed the global Hamiltonian operator for 2D-MPHOP, involving three fundamental parts: the first one is the ordinary Hamiltonian operator, in commutative quantum mechanics (CQM); the second part is the spin-orbit operator $H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)$, while the third one is the modified Zeeman operator $H_{\text{z-ph}}\left(r,\chi,\ \bar{\sigma}\right)$ and corresponding energy eigenvalues by applying the perturbation method. Furthermore, we have shown that the global quantum group (GQG) of (NC: 2D-RSP) symmetries has been broken automatically and replaced by subgroup (NC: 2D-RS) under 2D-MPHOP molecules interactions. We find the energy levels of the studied homonuclear and heteronuclear diatomic molecules in CQM as special case, when we use the simultaneously two limits $\left(\theta,\bar{\theta}\right)\to\left(0,0\right)$.

Keywords: Two dimensional Schrödinger equation, Pseudoharmonic potential, Noncommutative space-phase, The Moyal-Weyl product.

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1. INTRODUCTION

Schrodinger equation (SE) is one of the most powerful tools to describe the physical and chemical phenomena in nonrelativistic quantum mechanics and its extension. In recent years, there have been several studies of the bound states of molecules, using SE, within a compound harmonic oscillator potential and its inverse potential, which is known by the pseudoharmonic oscillator potential (PHOP). The PHOP is one of the important central model potentials, and it has been a subject of interest in many fields of chemical and physical fields, molecular physics, it has been used to describe the roto-vibrational states of homonuclear (O_2, N_2 and H_2) and heteronuclear (CH and ScH) diatomic molecules. Furthermore, this potential may be used for the energy spectrum of linear and non-linear systems. As known, it first appeared in Gol'dman et *al.* paper in 1960 [1-4]. Recently, some authors have focused on extension of SE to the new space-time, which gives more detail about the systems under study. And in view of what has been mentioned, we would like to study the results of the interactions of these potentials in a large space and phase of quantum mechanics, known by the noncommutative quantum mechanics (NCQM) or extended quantum mechanics (EQM), which known firstly by Heisenberg and was developed by Snyder at 1947. Motivated by these, over the past few years, theoretical physicists have shown a great deal of interest in solving the fundamental equations for various potentials in NCQM to obtain profound interpretations at microscopic scale [5-9] and in particularly, our previous works in the case of (NC: 2D-RSP) [10, 11], in (NC: 3D-RSP) [12, 13] and in relativistic EQM [14, 15]. The concepts of noncommutativity of space and phase developed using notions of the Moyal-Weyl product (*- product), which modifies the ordinary product of two arbitrary functions $\left(fg\right)\left(x,p\right)$ to the form $\left(f*g\right)\left(x,p\right)$ at first order of two infinitesimal antisymmetric parameters ($\theta,\bar{\theta}$) as (throughout this paper, the atomic units i.e. $c=\hbar=1$ are employed) [5-8]:

$$\begin{aligned}&\left(f*g\right)\left(x,p\right)=\left(fg\right)\left(x,p\right)-\\&-\frac{i}{2}\left(\theta^{\mu\nu}\partial_{\mu}^{x}f\,\partial_{\nu}^{x}g+\bar{\theta}^{\mu\nu}\partial_{\mu}^{p}f\,\partial_{\nu}^{p}g\right)\left(x,p\right)\end{aligned} \tag{1}$$

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[*] abmaireche@gmail.com

Here $2\left(\theta^{\mu\nu},\bar{\theta}^{\mu\nu}\right)\equiv\varepsilon^{\alpha\mu\nu}\left(\theta_{\alpha},\bar{\theta}_{\alpha}\right)$ denotes two antisymmetric constant tensors. Eq. (1) presents the noncommutativity effects of space and phase, which allow us to obtain the following non null commutators for NC coordinate and momentum $\left(\hat{x}_{\mu},\hat{p}_{\mu}\right)$ in GQG of (NC: 2D-RSP) symmetries as follows [9-12]:

$$\begin{cases}\left[\hat{x}_{\mu}\overset{*}{,}\hat{p}_{\nu}\right]=\left[\hat{x}_{\mu}(t)\overset{*}{,}\hat{p}_{\nu}(t)\right]=i\delta_{\mu\nu}\Rightarrow\\ \Delta\hat{x}_{\mu}\Delta\hat{p}_{\nu}\equiv\Delta\hat{x}_{\mu}(t)\Delta\hat{p}_{\nu}(t)\geq\dfrac{\delta_{\mu\nu}}{2}\\ \left[\hat{x}_{\mu}\overset{*}{,}\hat{x}_{\nu}\right]=\left[\hat{x}_{\mu}(t)\overset{*}{,}\hat{x}_{\nu}(t)\right]=i\theta_{\mu\nu}\Rightarrow\\ \Delta\hat{x}_{\mu}\hat{x}_{\nu}\equiv\Delta\hat{x}_{\mu}(t)\hat{x}_{\nu}(t)\geq\dfrac{\left|\theta_{\mu\nu}\right|}{2}\\ \left[\hat{p}_{\mu}\overset{*}{,}\hat{p}_{\nu}\right]=\left[\hat{p}_{\mu}(t)\overset{*}{,}\hat{p}_{\nu}(t)\right]=i\bar{\theta}_{\mu\nu}\Rightarrow\\ \Delta\hat{p}_{\mu}\Delta\hat{p}_{\nu}\equiv\Delta\hat{p}_{\mu}(t)\Delta\hat{p}_{\nu}(t)\geq\dfrac{\left|\bar{\theta}_{\mu\nu}\right|}{2}\end{cases}\qquad(2)$$

On the other hand, although the 2D-MPHOP for previous diatomic molecules has attracted wide attention, this is not the case for the 2D and 3D MPHOP for one-electron atoms. The 2D and 3D MPHOP for one-electron atoms have been studied in our references [16-18]. The principal goal of this work is on focusing around to the extend our works from NC: 2D-RSP and NC: 3D-RSP models for one electron atoms to NC: 2D-RSP model for some diatomic molecules, which we have mentioned previously based on the Ref. [2] to find out what will happen with nonrelativistic spectrum if effects of 2D noncommutativity of space and phase are considered for 2D-MPHOP. However, the solutions of deformed radial Schrodinger equation for any angular momentum quantum number *l*, with 2D-MPHOP, for diatomic molecules O_2, N_2, H_2, CH, and ScH have not yet been reported. The content of the present study is regulated as follows. After this introduction, in the second section we briefly review the SE with 2D-PHOP and we convert the mechanical properties to corresponding atomic properties. Next, we shall briefly explain the fundamental concepts of the generalized Bopp's shift method, and then we derive the 2D-MPHOP and deformed spin-orbital Hamiltonian operator $H_{so-ph}\left(r,\theta,\bar{\theta}\right)$ for previous diatomic molecules under 2D-NPHOP. In the next step, we apply the standard perturbation theory to find the corresponding spectrum energy $E_{\text{so-ph}}\left(n_r,j,l,s\right)$ for n^{th} excited states and then we end this section deducing the magnetic spectrum $E_{z-ph}\left(n_r,r_e,D_e,m\right)$ produced automatically by the external magnetic field. In section 4, we summarise the global spectrum for diatomic molecules O_2, N_2, H_2, CH, and ScH under 2D-MPHOP and derive the corresponding deformed Hamiltonian operator $H_{nc-ph}\left(r,\theta,\bar{\theta},\chi,\bar{\sigma}\right)$ in EQM. Finally, in section 5, we give a brief conclusion to finalize the paper.

2. REVIEW OF THE SPECTRUM OF 2D-PHOP IN ORDINARY QUANTUM MECHANICS

Let us present a brief review of the ordinary energy eigenvalues $E_{n_r l}$ and the normalized wave functions $\Psi_{n_r lm}(r,\phi)=R_{nl}(r)exp(\pm im\phi)$ for 2D-PHOP. Firstly, the radial part $R_{n_r l}(r)$ for 2D Schrödinger equation (2D-SE) satisfies the following equation [2]:

$$\begin{aligned}&\frac{d^2R_{n_r l}(r)}{dr^2}+\frac{1}{r}\frac{dR_{n_r l}(r)}{dr}+\\&2\mu\left(E_{n_r l}-V(r)-\frac{l^2}{2\mu r^2}\right)R_{n_r l}(r)=0\end{aligned}\qquad(3)$$

where $\mu\equiv\dfrac{m_1m_2}{m_1+m_2}$, $(n_r=0,1,....)$ and $l=\overline{0,n_r-1}$ are the reduced mass of diatomic molecules, the principal quantum and orbital angular momentum quantum numbers, respectively, while the 2D-PHOP is given by [2-3]:

$$V(r)=\frac{1}{8}kr_0^{\,2}\left(\frac{r}{r_0}-\frac{r_0}{r}\right)^2\equiv D_e\left(\frac{r}{r_e}-\frac{r_e}{r}\right)^2=Ar^2+\frac{B}{r^2}+c\,.\qquad(4)$$

We make two simultaneous translations $\frac{1}{8}kr_0^{\,2}\to D_e$ and $r_0\to r_e$, which are the dissociation energy (*k* is the force constant) and equilibrium intermolecular separation (r_0 is the equilibrium bond length). Thus we obtain $A=D_e/r_e^2$, $B=D_er_e$ and $c=-2D_e$. According to [2], the complete orthonormalized wave function $\Psi_{n_r lm}(r,\phi)$ for 2D-PHOP is determined from the following equation:

$$\begin{aligned}&\Psi_{n_r lm}(r,\phi)=C_{n_r l}r^{\mu_l}\,exp\left(-\lambda r^2\right)L_{n_r}^{\mu_l}\left(2\lambda r^2\right)\times\\&\times\left(2\lambda r^2\right)exp(\pm im\phi)\end{aligned}\qquad(5)$$

where $C_{n_r,l}=\left[\dfrac{\left(2\lambda^2\right)^{\left(\mu_l+1\right)}n_r!}{\Gamma\left(n_r+\mu_l+1\right)}\right]^{1/2}$ and $L_n^{\mu_l}\left(2\lambda r^2\right)$ are the associated Laguerre functions. Therefore, the energy eigenvalues $E_{n_r l}$ of this potential in 2D-space are

$$E_{n_r l}=\frac{1}{2}(n_r+1)\sqrt{\frac{k}{\mu}}-\frac{kr_0^{\,2}}{4}\equiv\frac{1}{2}(n_r+1)\sqrt{\frac{8D_e}{\mu r_e^{\,2}}}-2D_e\,,\qquad(6)$$

where the two factors λ and μ_l are determined from the two projection expressions:

$$\lambda=\sqrt{\frac{\mu D_e}{8r_e^{\,2}}}\equiv\sqrt{\frac{\mu k}{16}}\text{ and }\mu_l=\sqrt{l^2+\mu kr_0^{\,4}/4}\,.\qquad(7)$$

Thus, we have transformed the mechanical properties (k,r_0), which appear in [2], to the atomic properties

(D_e, r_e) in addition to the orthonormalized wave function $\Psi_{n_r lm}(r,\phi)$ and the energy eigenvalues $E_{n_r l}$ for previous diatomic molecules under 2D-PHOP.

3. THEORETICAL FRAMEWORK

3.1 Theoretical Description of the Generalized Bopp's Shift Method in 2D Spaces-phases

In order to obtain 2D-DSE in EQM, we replace ordinary Hamiltonian operator $\hat{H}(p_\mu, x_\nu)$, ordinary complex function $\Psi_{n_r lm}(r,\phi)$, ordinary energy $E_{n_r l}$ and ordinary product by NC Hamiltonian operator $\hat{H}_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)$, complex function $\hat{\Psi}(\vec{\hat{r}})$, energy E_{nc-ph} and the Moyal-Weyl product (*-product), respectively. Let us write the 2D-DSE for diatomic molecules under 2D-MPHOP as follows [9-12]:

$$\begin{aligned} &\hat{H}(p_\mu, x_\nu)\Psi_{n_r lm}(r,\phi) = E_{n_r l}\Psi_{n_r lm}(r,\phi) \\ &\Rightarrow \hat{H}_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu) * \hat{\Psi}(\vec{\hat{r}}) = E_{nc-ph}\hat{\Psi}(\vec{\hat{r}}) \end{aligned} \tag{8}$$

The NC Hamiltonian operator $\hat{H}_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)$ acts by the Moyal-Weyl product on the corresponding complex wave function $\hat{\Psi}(\vec{\hat{r}})$ of the new system to give us the energy eigenvalues E_{nc-ph} of the new system energy in EQM. In the EQM, the Hamiltonian operator $\hat{H}_{nc-ph}(\hat{p}_i, \hat{x}_i)$ for diatomic molecules under 2D-MPHOP can be resumed in three physical varieties, the first one is $\hat{H}_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)$ in (NC: 2D-RSP), the second is $\hat{H}_{nc-ph}(p_\mu, \hat{x}_\nu)$ in (NC: 2D-RS) symmetries, while the third one is $\hat{H}_{nc-ph}(\hat{p}_\mu, x_\nu)$ (NC: 2D-RP), respectively [13-15]:

$$\hat{H}_{nc-ph}(\hat{p}_\alpha, \hat{x}_\beta) \equiv \hat{H}\left(\hat{p}_\alpha = p_\alpha + \frac{\bar{\theta}_{\alpha\beta}}{2}x_\beta; \hat{x}_\alpha = x_\alpha - \frac{\theta_{\alpha\beta}}{2}p_\beta\right) \quad \text{for} \quad \text{(NC: 2D-RSP)} \tag{9.1}$$

$$\hat{H}_{nc-ph}(\hat{p}_\alpha, \hat{x}_\beta) \equiv \hat{H}\left(\hat{p}_\alpha = p_\alpha + \frac{\bar{\theta}_{\alpha\beta}}{2}x_\beta; \hat{x}_\alpha = x_\alpha\right) \quad \text{for} \quad \text{(NC: 2D-RP)} \tag{9.2}$$

$$\hat{H}_{nc-ph}(\hat{p}_\alpha, \hat{x}_\beta) \equiv \hat{H}\left(\hat{p}_\alpha = p_\alpha; \hat{x}_\alpha = x_\alpha - \frac{\theta_{\alpha\beta}}{2}p_\beta\right) \quad \text{for} \quad \text{(NC: 2D-RS)} \tag{9.3}$$

To find the analytical solutions of the Eq. (8) we must apply the generalized Bopp's shift method instead of solving the 2D-DSE for 2D-MPHOP directly with Moyal-Weyl product; we treated by applying directly the usual commutators on quantum mechanics, in addition to the commutators $[\hat{x}_\alpha, \hat{x}_\beta]$ and $[\hat{p}_\alpha, \hat{p}_\beta]$ due to (space-phase) noncommutativity [15-16]:

$$[\hat{x}_\alpha, \hat{x}_\beta] = i\theta_{\alpha\beta} \text{ and } [\hat{p}_\alpha, \hat{p}_\beta] = i\bar{\theta}_{\alpha\beta}\,(\alpha, \beta = 1,2) \tag{10}$$

It is well known that the two operators $\hat{x}_\alpha$ and $\hat{p}_\beta$ are given by the following Darboux transformations [14-17]:

$$\hat{x}_\alpha = x_\alpha - \frac{\theta_{\alpha\beta}}{2}p_\beta \text{ and } \hat{p}_\alpha = p_\alpha + \frac{\bar{\theta}_{\alpha\beta}}{2}x_\beta\,(\alpha, \beta = 1,2) \tag{11}$$

The two ordinary variables (x_α, p_β) play the same role as in CQM and obey the usual commutation relations

$$[x_\alpha, p_\beta] = [x_\alpha(t), p_\beta(t)] = i\delta_{\alpha\beta j},$$
$$[x_\alpha, x_\beta] = [x_\alpha(t), x_\beta(t)] = 0 \quad \text{and}$$
$$[p_\alpha, p_\beta] = [p_\alpha(t), p_\beta(t)] = 0.$$

In recent work, we are interested in the first variety that appears in Eq. (9.1). As direct consequences of the generalized Bopp's method (modified by a shift), the 2D-DSE for studied diatomic molecules under 2D-MPHOP reduces the 2D-SE with two translations in space and momentum:

$$\begin{aligned} &\hat{H}_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu) * \hat{\Psi}(\vec{\hat{r}}) = E_{nc-ph}\hat{\Psi}(\vec{\hat{r}}) \\ &\Rightarrow H_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)\psi(\vec{r}) = E_{nc-ph}\psi(\vec{r}) \end{aligned} \tag{12}$$

The Hamiltonian operator $H_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)$ that appears above can be determined from the following relation:

$$H_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu) = \frac{\hat{p}^2}{2\mu} + A\hat{r}^2 + \frac{B}{\hat{r}^2} + c\,. \tag{13}$$

According to our previous references [16, 17], we can determine the two operators $\hat{r}^2$ and $\hat{p}^2$ in EQM from the following equation:

$$\hat{r}^2 = r^2 - L_z\theta + O(\theta^2) \text{ and } \hat{p}^2 = p^2 + L_z\bar{\theta} + O(\bar{\theta}^2) \tag{14}$$

with $(\theta, \bar{\theta}) \equiv (\theta_{12}, \bar{\theta}_{12})$, $L_x = L_y = 0$, $r^2 = x^2 + y^2$, $p^2 = p_x{}^2 + p_y{}^2$ and $L_z = xp_y - yp_x$. After straightforward calculations, one can obtain the important term ($\frac{1}{\hat{r}^2}$), which will be used to determine the NC Hamiltonian operator $H_{nc-ph}(\hat{p}_\mu, \hat{x}_\nu)$ in GQG of NC: 2D-RSP symmetries as follows:

$$\frac{1}{\hat{r}^2} = \frac{1}{r^2} + \frac{L_z\theta}{r^4} + O(\theta^2). \tag{15}$$

Substituting equations (14) and (15) into Eq. (13), one gets the 2D-NC $H_{nc-ph}\left(\hat{p}_\mu,\hat{x}_\mu\right)$ in GQG of NC: 2D-RSP symmetries as follows:

$$H_{nc-ph}\left(\hat{p}_\mu,\hat{x}_\nu\right)=H_{ph}\left(p_\mu,x_\nu\right)+H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right), \quad (16)$$

where $H_{ph}\left(p_\mu,x_\nu\right)$ and $H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)$ are given by:

$$H_{ph}\left(p_\mu,x_\nu\right)=\frac{p^2}{2\mu}+Ar^2+\frac{B}{r^2}+c\,, \quad (17)$$

$$H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)=\left(\frac{B}{r^4}-A\right)L_z\theta+\frac{L_z\bar{\theta}}{2\mu}+O\left(\theta^2,\bar{\theta}^2\right) \quad (18)$$

It is clear that the operator $H_{ph}\left(p_\mu,x_\nu\right)$ is just the Hamiltonian operator for diatomic molecules in ordinary quantum mechanics while the generated part $H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)$ appears as results of deformation of noncommutativity space phase. In recent work, we can disregard the second term in $H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)$ because we are interested in the corrections of first order θ and $\bar{\theta}$.

3.2 2D Spin-orbit Hamiltonian Operators for Diatomic Molecules under 2D-MEPHP

In this subsection, we want to derive the physical form of the induced Hamiltonian $H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)$ due to space-phase noncommutativity. To achieve this goal, we replace both $L_z\theta$ and $L_z\bar{\theta}$ by useful physical forms $\alpha\theta\vec{S}\vec{L}$ and $\alpha\bar{\theta}\vec{S}\vec{L}$, respectively [16-18]:

$$H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)\equiv H_{\text{pert-ph}}\left(r,\theta,\bar{\theta}\right)= -\alpha\left\{\frac{D_e r_e^2}{r^4}-\frac{D_e}{r_e^2}+\frac{\bar{\theta}}{2\mu}\right\}\vec{\mathbf{L}}\vec{S} \quad (19)$$

Here α is the atomic fine structure constant, $\vec{S}$ denotes the spin of diatomic molecules O2, N2, H2, CH and ScH, thus, the spin-orbit interactions $H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)$ appear automatically. Now, physically, we can rewrite the quantum spin-orbit coupling $\vec{\mathbf{L}}\vec{S}$ as follows:

$$\vec{J}=\vec{L}+\vec{S}\Rightarrow 2\vec{L}\vec{S}=\vec{J}^2-\vec{L}^2-\vec{S}^2\,. \quad (20)$$

Here $\vec{J}$ is the total momentum of the studied diatomic molecule. Substitution of this equation into (19) yields:

$$H_{\text{pert-kp}}\left(r,\theta,\bar{\theta}\right)=-\frac{\alpha}{2}\left\{\frac{D_e r_e^2}{r^4}-\frac{D_e}{r_e^2}+\frac{\bar{\theta}}{2\mu}\right\}\left(\vec{J}^2-\vec{L}^2-\vec{S}^2\right). \quad (21)$$

In quantum mechanics, the eigenvalues $k(j,l,s)$ of the spin-orbit coupling $\vec{\mathbf{L}}\vec{S}$ are equal to $\frac{1}{2}\left[j(j+1)-l(l+1)-s(s+1)\right]$ and the eigenvalues of the total operator $\vec{J}$ are:

$$j=\underbrace{|l-s|,\ |l-s|+1,...0,....|l+s|-1,|l+s|}_{N-\text{values}},$$

which are obtained in the interval $|l-s|\le j\le|l+s|$. After straightforward calculation, the radial functions $R_{n_r l}(r)$ satisfy the following differential equation in EQM for diatomic molecules under 2D-MPHOP:

$$\frac{d^2R_{n_r l}(r)}{dr^2}+\frac{1}{r}\frac{dR_{n_r l}(r)}{dr}+2\mu\left(E_{nc-ph}+\frac{D_e}{r_e^2}r^2+\frac{D_e r_e^2}{r^2}-2D_e-\alpha\left\{\frac{D_e r_e^2}{r^4}-\frac{D_e}{r_e^2}+\frac{\bar{\theta}}{2\mu}\right\}\vec{\mathbf{L}}\vec{S}-\frac{l^2}{2\mu r^2}\right)R_{n_r l}(r)=0\,. \quad (22)$$

We have seen previously that the induced spin-orbit terms $H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)$ are very infinitesimal compared to the principal Hamiltonian operator $H_{ph}(p,x)$ in ordinary quantum mechanics for diatomic molecules under 2D-PHOP. This allows applying standard perturbation theory to determine the nonrelativistic energy corrections $E_{ph}\left(n_r,j,l,s\right)$ of diatomic molecules at first order of two infinitesimal parameters θ and $\bar{\theta}$ due to noncommutativity space phase.

3.3 Bound State Solution for Spin-orbit Operator for 2D-MPHOP

The principal goal of this subsection is to determine the energy spectrum $E_{so-ph}\left(n_r,j,l,s\right)$ corresponding to $H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)$ by applying standard perturbation theory at first order of θ and $\bar{\theta}$ and through the structure constants which specified the dimensionality of 2D-MPHOP of diatomic molecules such as O2, N2, H2, CH and ScH. Thus, we obtain the following results of modified energy:

$$E_{so-ph}\left(n_r,j,l,s\right)=N(n)k(j,l,s)\int_0^{+\infty} r^{2\mu_l}\,exp\left(-2\lambda r^2\right)\left[L_{n_r}^{\mu_l}\left(2\lambda r^2\right)\right]^2\left\{\theta\left(\frac{D_e r_e^2}{r^4}-\frac{D_e}{r_e^2}\right)+\frac{\bar{\theta}}{2\mu}\right\}dr \quad (23)$$

with $N(n_r,l)$ equal to the values $\prod\frac{\left(2\lambda^2\right)^{(\mu_l+1)}n_r!}{\Gamma\left(\mathrm{n_r}+\mu_l+1\right)}$. In view of the transformation $r^2\equiv t$, Eq. (23) becomes as follows:

$$E_{\text{ph}}\left(n_r,j,l,s\right)=N(n,l)k(j,l,s)\int_0^{+\infty} t^{2\mu_l}\,exp\left(-2\lambda t\right)\left[L_n^{\mu_l}\left(2\lambda t\right)\right]^2\left\{\theta\left(\frac{D_e r_e^2}{t^2}-\frac{D_e}{r_e^2}\right)+\frac{\bar{\theta}}{2\mu}\right\}dt\,. \quad (24)$$

If we introduce the following three factors $T_i\left(n,r_e,D_e\right)\left(i=\overline{1,3}\right)$ as:

$$T_1\left(n_r,r_e,D_e\right)\equiv D_e r_e^{\,2}\int_0^{+\infty} t^{\left(2\mu_l-1\right)-1}exp\left(-2\lambda t\right)\left[L_{n_r}^{\mu_l}\left(2\lambda t\right)\right]^2 dt,$$
$$T_3\left(n_r,r_e,D_e\right)\ \equiv\int_0^{+\infty} t^{\left(2\mu_l+1\right)-1}exp\left(-2\lambda t\right)\left[L_{n}^{\mu_l}\left(2\lambda t\right)\right]^2 dt \qquad (25)$$
$$T_2\left(n_r,r_e,D_e\right)\equiv-\frac{D_e}{r_e^{\,2}}T_3\left(n_r,r_e,D_e\right)$$

on arranging Eq. (24), we obtain our nonrelativistic energy corrections $E_{\text{so-ph}}\left(n_r,j,l,s\right)$ at first order of two infinitesimal parameters θ and $\bar{\theta}$ for the previous diatomic molecules as:

$$E_{\text{so-ph}}\left(n_r,j,l,s\right)=N\left(n_r,l\right)k\left(j,l,s\right)k\left(j,l,s\right)$$
$$\left\{\theta\sum_{i=1}^{2}T_i\left(n_r,r_e,D_e\right)+\frac{\bar{\theta}}{2\mu}T_3\left(n_r,r_e,D_e\right)\right\} \qquad (26)$$

To obtain the exact results of the three terms $T_i\left(n_r,r_e,D_e\right)$, $\left(i=\overline{1,3}\right)$, we apply the following special integral of hypergeometric function [20]:

$$\int_0^{+\infty} t^{\alpha-1.}_{\cdot}\,exp\left(-\delta t\right)L_m^{\eta}\left(\delta t\right)L_n^{\beta}\left(\delta t\right)dt=$$
$$=\frac{\delta^{-\alpha}\Gamma\left(n-\alpha+\beta+1\right)\Gamma\left(m+\eta+1\right)}{m!n!\Gamma\left(1-\alpha+\beta\right)\Gamma\left(1+\eta\right)}\times \qquad (27)$$
$$\times{}_3F_2\left(-m,\alpha,\alpha-\beta;-n+\alpha,\eta+1;1\right)$$

The hypergeometric function ${}_3F_2\left(-m,\alpha,\alpha-\beta;-n+\alpha,\lambda+1;1\right)$ is a particular case of the generalized hypergeometric series ${}_qF_p\left(-m,\alpha,\alpha-\beta;-n+\alpha,\lambda+1;1\right)$, when $p=2$ and $q=3$. After straightforward calculations, we obtain the three factors $T_i\left(n_r,r_e,D_e\right)\left(i=\overline{1,3}\right)$ as follows:

$$T_1\left(n_r,r_e,D_e\right)\equiv D_e r_e^{\,2}\frac{\left(2\lambda\right)^{-\left(2\mu_l-1\right)}\Gamma\left(n_r-\mu_l+2\right)\Gamma\left(n_r+\mu_l+1\right)}{n_r!^2\Gamma\left(2-\mu_l\right)\Gamma\left(1+\mu_l\right)}\times{}_3F_2\left(-n_r,2\mu_l-1,\mu_l-1;-n_r+2\mu_l-1,\eta+1;1\right)$$
$$T_3\left(n_r,r_e,D_e\right)\ \equiv\frac{\left(2\lambda\right)^{-\left(2\mu_l+1\right)}\Gamma\left(n_r-\mu_l\right)\Gamma\left(n_r+\mu_l+1\right)}{n_r!^2\Gamma\left(-\mu_l\right)\Gamma\left(1+\mu_l\right)}\times{}_3F_2\left(-n_r,2\mu_l+1,\mu_l+1;-n_r+2\mu_l+1,\mu_l+1;1\right) \qquad (28)$$

Regarding Eq. (7), μ_l is positive, thus we have $\Gamma\left(-\mu_l\right)=\infty$, then, the two factors $T_2\left(n_r,r_e,D_e\right)\equiv-\frac{D_e}{r_e^{\,2}}T_3\left(n_r,r_e,D_e\right)=0$.

Further, the substitution of Eq. (28) into Eq. (26) enables us to obtain the first quantum correction $E_{so-ph}\left(n_r,j,l,s\right)$ of energy levels of all bound states as:

$$E_{\text{so-ph}}\left(n_r,j,l,s\right)=\theta N\left(n_r,l\right)k\left(j,l,s\right)D_e r_e^{\,2}\frac{\left(2\lambda\right)^{-\left(2\mu_l-1\right)}\Gamma\left(n_r-\mu_l+2\right)\Gamma\left(n_r+\mu_l+1\right)}{n_r!^2\Gamma\left(2-\mu_l\right)\Gamma\left(1+\mu_l\right)}\times{}_3F_2\left(-n_r,2\mu_l-1,\mu_l-1;-n_r+2\mu_l-1,\mu_l+1;1\right) \qquad (29)$$

Thus, the EQM of noncommutative two-dimensional real space-phase is reduced to the sub-group symmetry of noncommutative two-dimensional real space for diatomic molecules under 2D-MPHOP. Allow us to obtain the following important physical results:

$$H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)\Psi_{n_r lm}\left(r,\phi\right)=E_{so-ph}\left(n_r,j,l,s\right)\Psi_{n_r lm}\left(r,\phi\right) \qquad (30)$$

3.4 Bound State Solution for Modified Zeeman Effect for 2D-MPHOP

In this subsection, it is possible to obtain the second automatically symmetry for diatomic molecules O_2, N_2, H_2, CH and ScH under 2D-MPHOP. This physical phenomenon is induced of the influence of an external uniform magnetic field $\vec{\aleph}$, if we make the following two simultaneous transformations to ensure that previous calculations are not reputed:

$$\left(\theta,\bar{\theta}\right)\rightarrow\left(\chi,\ \bar{\sigma}\right)\aleph. \qquad (31)$$

Here χ and $\bar{\sigma}$ are just two infinitesimal real proportional constants, and to simplify calculations without compromising physical content we choose the magnetic field $\vec{\aleph}=\aleph\vec{k}$. Then we transform the spin-orbit coupling $\frac{\alpha}{2}\left\{\theta\left(\frac{D_e r_e^{\,2}}{r^4}-\frac{D_e}{r_e^{\,2}}\right)+\frac{\bar{\theta}}{2\mu}\right\}L_z$ to this new physical phenomena as follows:

$$\frac{\alpha}{2}\left\{\theta\left(\frac{D_e r_e^{\,2}}{r^4}-\frac{D_e}{r_e^{\,2}}\right)+\frac{\bar{\theta}}{2\mu}\right\}L_z\rightarrow$$
$$\left(\chi\left(\frac{D_e r_e^{\,2}}{r^4}-\frac{D_e}{r_e^{\,2}}\right)+\frac{\bar{\sigma}}{2\mu}\right)\aleph L_z \qquad (32)$$

This allowed to derive the modified magnetic Hamiltonian operator $H_{\text{z-ph}}\left(r,\chi,\ \bar{\sigma}\right)$ for previous diatomic molecules under 2D-MPHOP in global (NC: 2D-RSP) symmetries as:

$$H_{\text{z-ph}}\left(r,\chi,\ \bar{\sigma}\right)=\left(\chi\left(\frac{D_e r_e^{\,2}}{r^4}-\frac{D_e}{r_e^{\,2}}\right)+\frac{\bar{\sigma}}{2\mu}\right)\left(\vec{\aleph}\vec{J}-\vec{S}\vec{\aleph}\right) \qquad (33)$$

where $\left(-\vec{S}\vec{\aleph}\right)$ presents the ordinary Hamiltonian of Zeeman effect for 2D-PHOP. To determine the exact NC magnetic modifications of the modified energy

$E_{\text{z-pd}}\left(n_r, r_e, D_e, m\right)$ corresponding to above operator for 2D-MPHOP, we make the two simultaneous transformations $k(j,l,s) \to m$ (with $-l \le m \le +l$) and $\theta \to \chi$ in the Eq. (28) to get the following results:

$$E_{\text{z-ph}}\left(n_r, r_e, D_e, m\right) = \theta N\left(n_r, l\right) m D_e r_e^{2} \frac{(2\lambda)^{-\left(2\mu_l - 1\right)} \Gamma\left(n_r - \mu_l + 2\right) \Gamma\left(n_r + \mu_l + 1\right)}{n_r!^{2} \Gamma\left(2 - \mu_l\right) \Gamma\left(1 + \mu_l\right)} \times {}_3F_2\left(-n_r, 2\mu_l - 1, \mu_l - 1; -n_r + 2\mu_l - 1, \mu_l + 1; 1\right) \aleph \tag{34}$$

We end this subsection by addressing the important results:

$$\begin{aligned} &H_{\text{z-ph}}\left(r, \theta, \bar{\theta}\right) \Psi_{n_r l m}(r, \phi) = \\ &E_{\text{z-ph}}\left(n_r, r_e, D_e, m\right) \Psi_{n_r l m}(r, \phi) \end{aligned} \tag{35}$$

4. RESULTS AND DISCUSSION OF GLOBAL SPECTRUM FOR 2D-MPHOP IN EQM

In the previous subsections, we have solved the 2D-DSE for diatomic molecules, such as O₂, N₂, H₂, CH and ScH, under the influence of 2D-MPHOP and obtained the two important values of the energy eigenvalues $E_{\text{so-ph}}\left(n_r, j, l, s\right)$ and $E_{\text{z-ph}}\left(n_r, r_e, D_e, m\right)$ corresponding to two induced operators $H_{\text{so-ph}}\left(r, \theta, \bar{\theta}\right)$ and $H_{\text{z-ph}}\left(r, \chi, \bar{\sigma}\right)$, respectively. In what follows, we resume the obtained results of the modified energy levels $E_{\text{nc -ph}}\left(n_r, j, l, s, m\right)$ of studied molecules, the ordinary values of energy (6). In addition to the two new original results (29) and (34), the explicit bound state energies $E_{\text{nc -ph}}\left(n_r, j, l, s, m\right)$ for 2D-MPHOP take the form:

$$\begin{aligned} E_{\text{nc -ph}}\left(n_r, j, l, s, m\right) = {} & \tfrac{1}{2}\left(n_r + 1\right) \sqrt{\frac{8D_e}{\mu r_e^{2}}} - 2D_e + N\left(n_r, l\right) m D_e r_e^{2} \frac{(2\lambda)^{-\left(2\mu_l - 1\right)} \Gamma\left(n_r - \mu_l + 2\right) \Gamma\left(n_r + \mu_l + 1\right)}{n_r!^{2} \Gamma\left(2 - \mu_l\right) \Gamma\left(1 + \mu_l\right)} \times \\ & F_2\left(-n_r, 2\mu_l - 1, \mu_l - 1; -n_r + 2\mu_l - 1, \mu_l + 1; 1\right) \left\{\theta k(j, l, s) + \chi \aleph m\right\} \end{aligned} \tag{36}$$

Thus, the total energy $E_{\text{nc-ph}}\left(n_r, j, l, s, m\right)$ for 2D-MPHOP in EQM is the sum of the ordinary part of energy $E_{n_r l}$ and the two corrections of energy $E_{\text{so-ph}}\left(n_r, j, l, s\right)$ and $E_{\text{z-ph}}\left(n_r, r_e, D_e, m\right)$. This is one of the main motivations for the topic of this search work. Because our obtained eigenvalues of energies $E_{\text{nc -ph}}\left(n_r, j, l, s, m\right)$ are real, this allows us to consider the deformed diagonal Hamiltonian $H_{nc-ph}\left(r, \theta, \bar{\theta}, \chi, \bar{\sigma}\right)$ as a Hermitian operator, and based on the previous obtained results (see two equations (19) and (33)), the Hamiltonian operator for 2D-MPHOP for studied diatomic molecules takes the form at first order in θ and $\bar{\theta}$ as:

$$\begin{aligned} &H_{nc-ph}\left(r, \theta, \bar{\theta}, \chi, \bar{\sigma}\right) = \boldsymbol{H}_{ph}\left(r, \theta, \bar{\theta}, \chi, \bar{\sigma}\right) + \\ &H_{so-ph}\left(r, \theta, \bar{\theta}\right) + H_{\text{z-ph}}\left(r, \chi, \bar{\sigma}\right) \end{aligned} \tag{37}$$

where the three parts $H_{ph}\left(r, D_e, r_e\right)$, $H_{\text{so-ph}}\left(r, \theta, \bar{\theta}\right)$ and $H_{\text{z-ph}}\left(r, \chi, \bar{\sigma}\right)$ are given by:

$$\begin{aligned} &H_{ph}\left(r, D_e, r_e\right) = -\frac{1}{2\mu}\left(\tfrac{1}{r} \tfrac{\partial}{\partial r}\left(r \tfrac{\partial}{\partial r}\right) + \tfrac{1}{r^2} \tfrac{\partial^2}{\partial \phi^2}\right) + \\ &+ \frac{D_e}{r_e^{2}} r^2 + \frac{D_e r_e^{2}}{r^2} - 2D_e \\ &H_{\text{so-ph}}\left(r, \theta, \bar{\theta}\right) = -\alpha\left\{\frac{D_e r_e^{2}}{r^4} - \frac{D_e}{r_e^{2}} + \frac{\bar{\theta}}{2\mu}\right\} \vec{\mathbf{L}} \vec{S} \\ &H_{\text{z-ph}}\left(r, \chi, \bar{\sigma}\right) = \left(\chi\left(\frac{D_e r_e^{2}}{r^4} - \frac{D_e}{r_e^{2}}\right) + \frac{\bar{\sigma}}{2\mu}\right)\left(\vec{\aleph} \vec{J} - \vec{S} \vec{\aleph}\right) \end{aligned} \tag{38}$$

which is the principal Hamiltonian operator for diatomic molecules O₂, N₂, H₂, CH and ScH under the influence of 2D-MPHOP in the symmetries of EQM. It should be pointed out that this treatment considers only first order terms in either θ or $\bar{\theta}$. Finally, we end this section by introducing the important result of this work as:

$$\begin{aligned} &\left\{H_{\text{ph}}(r) + H_{\text{so-ph}}\left(r, \theta, \bar{\theta}\right) + H_{\text{z-ph}}\left(r, \chi, \bar{\sigma}\right)\right\} \Psi_{n_r l m}(r, \phi) = \\ &\left\{E_{n_r l} + E_{\text{so-ph}}\left(n_r, r_e, j, l, s\right) + E_{\text{z-ph}}\left(n_r, r_e, D_e, m\right)\right\} \Psi_{n_r l m}(r, \phi) \end{aligned} \tag{39}$$

It is important to notice that the appearance of the spin $\vec{S}$ and total momentum operator $\vec{J} = \vec{L} + \vec{S}$ in recent work for molecules O₂, N₂, H₂, CH and ScH under the influence of 2D-MPHOP in the non-relativistic 2D-DSE indicates a validity of the obtained results at high energy, where the relativistic Dirac equation is applied. This gives a positive indication of the possibility to apply a recent study of various nanoparticles at nanoscales. It is quite instructive to consider the case of vanishing of the two parameters $\left(\theta, \bar{\theta}\right)$. All obtained results for Hamiltonian and energies are reduced to corresponding values in ordinary quantum mechanics.

5. CONCLUSIONS

In this paper, the values of energy levels $E_{\text{nc -ph}}\left(n_r, j, l, s, m\right)$ of diatomic molecules O₂, N₂, H₂, CH and ScH have been examined analytically under 2D-MPHOP in the case of EQM via the generalized Bopp's method and standard perturbation theory. We briefly summarize what has been achieved in this research work and comment on the outlook on future work that can follow this paper:

- We have reviewed the nonrelativistic 2D-PHOP for molecules O₂, N₂, H₂, CH and ScH and the generalized Bopp's method.

- Our approach allows us to re-derive Hamiltonian operators $H_{nc-ph}\left(r,\theta,\bar{\theta},\chi,\bar{\sigma}\right)$ (in addition to the principal part, it contains two new perturbative terms: the first part is spin-orbit interaction $H_{so-ph}\left(r,\theta,\bar{\theta}\right)$, while the second one is modified Zeeman effect $H_{\text{z-ph}}\left(r,\chi,\bar{\sigma}\right)$) and the corresponding energy eigenvalues $E_{\text{nc -ph}}\left(n_r,j,l,s,m\right)$.
- We hope to get some interesting new applications to nonrelativistic 2D-PHOP in the study of different fields of matter sciences like solid-state physics, the history of molecular structures and other interactions.

Our results obtained are in exact agreement with those obtained in previous works [16-19]. It should be noted that the results obtained in this research would be identical with corresponding results in ordinary quantum mechanics when the two parameters $\left(\theta,\bar{\theta}\right)$ are reduced to the values (0, 0).

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Розв'язок двовимірного рівняння Шредінгера в симетріях розширеної квантової механіки для модифікованого псевдогармонічного потенціалу: застосування до деяких двохатомних молекул

Abdelmadjid Maireche

Laboratory of Physics and Material Chemistry, Physics Department, Sciences Faculty, University of M'sila, M'sila, Algeria

Пошук розв'язків рівняння Шредінгера (SE) з моделями фізично мотивованих потенціалів призвів до відкриття нових фізичних і хімічних явищ. Наприклад, потенціал псевдогармонічного осцилятора (PHOP) має дуже цікаву історію: він часто використовується для обчислення нормалізації зв'язаних станів і енергетичних рівнів деяких двохатомних молекул. Це дослідження було розділене на дві частини. По-перше, ми перетворили механічні властивості, пов'язані з постійною силою, довжиною рівноважного зв'язку, ортонормованою хвильовою функцією та власними значеннями енергії, на відповідні атомні властивості, які включають енергію дисоціації, та рівноважне міжмолекулярне розділення з метою застосування до гомоядерних двохатомних молекул, таких як O_2, N_2 та H_2, і гетероядерних двохатомних молекул, таких як CH і ScH. По-друге, ми дослідили деякі аспекти модифікованого 2D-PHOP (2D-MPHOP) в некомутативній 2D реальній просторовій фазі (NC: 2D-RSP) через узагальнений метод зсуву Боппа в рамках параметрів, обумовлених (просторово-фазовою) некомутативністю $(\theta,\bar{\theta})$, за допомогою розв'язку 2D-деформованого SE (2D-DSE). Ми реконструювали глобальний оператор Гамільтона для 2D-MPHOP з трьома фундаментальними частинами: перша – звичайний оператор Гамільтона, в комутативній квантовій механіці (CQM); друга частина – спін-орбітальний оператор $H_{\text{so-ph}}\left(r,\theta,\bar{\theta}\right)$, а третя – модифікований зееманівський оператор $H_{\text{z-ph}}\left(r,\chi,\bar{\sigma}\right)$ і відповідні власні значення енергії за допомогою методу збурень. Крім того, ми показали, що глобальна квантова група (GQG) симетрій (NC: 2D-RSP) була автоматично розбита і замінена підгрупою (NC: 2D-RS) при взаємодіях молекул 2D-MPHOP. Ми знайшли енергетичні рівні досліджуваних гомоядерних і гетероядерних двохатомних молекул у CQM як особливий випадок, коли одночасно використовуємо два обмеження $\left(\theta,\bar{\theta}\right)\rightarrow\left(0,0\right)$.

Ключові слова: Двовимірне рівняння Шредінгера, Псевдогармонічний потенціал, Некомутативна просторова фаза, добуток Мояля-Вейля.