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Exact solution of the semiconfined harmonic oscillator model with a position-dependent effective mass

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Abstract. We present a new model of a one-dimensional non-relativistic canonical quantum harmonic oscillator which is semiconfined. Semiconfinement is achieved by replacing the constant effective mass with a mass that varies with position. The problem is exactly solvable and the analytic expression of the wavefunctions of the stationary states is expressed by means of generalized Laguerre polynomials. Surprisingly, the energy spectrum completely overlaps with the energy spectrum of the standard non-relativistic canonical quantum harmonic oscillator. In the limit when the semiconfinement parameter a goes to infinity, the wavefunctions also tend to the wavefunction of the standard oscillator in terms of Hermite polynomials.

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1 Introduction

The harmonic oscillator, restoring its displacement to the equilibrium position under the force $F = -kx$, can be considered as one of the most versatile problems of modern physics. The solution to this problem in classical mechanics is standard. The motion of the simple harmonic oscillator under the force F is a sinusoidal oscillation with some constant amplitude that defines the borders of the maximal oscillations for the classical problem [1]. The study of the same problem within quantum mechanics opens the door to different viewpoints. In the non-relativistic approximation to quantum mechanics, the Schrödinger equation for the harmonic oscillator can be solved exactly. Here, two well-known solutions to the one-dimensional non-relativistic quantum harmonic oscillator problem are known: in the canonical approach, one finds the discrete energy spectrum with ground state level $\frac{1}{2}\hbar\omega$ and wavefunctions of the stationary states expressed by the Hermite polynomials [2]; in the non-canonical approach, one finds a discrete energy spectrum with ground state level $a\hbar\omega$ ($a \geq \frac{1}{2}$) and wavefunctions of the stationary states expressed by the generalized Laguerre polynomials [3]. It is obvious that canonical approach to the harmonic oscillator problem is simply one of the special cases of the same problem under the non-canonical approach, when $a = \frac{1}{2}$ [4,5].

Inspired by the solution of the (non-canonical) non-relativistic quantum oscillator in terms of generalized Laguerre polynomials, we decided to explore other possibilities to achieve exact solutions of the harmonic oscillator wavefunctions in terms of these polynomials. We achieved this goal by considering the non-relativistic quantum harmonic oscillator in the canonical approach, with wavefunctions vanishing from the left side at some finite value of the position x and from the right side at infinity. Due to such a property, we call this model the semiconfined quantum harmonic oscillator. Despite the fact that such an oscillator model has not been studied before theoretically, it can be a powerful tool for the description of a number of physical phenomena. For example, the growth of a monocrystal on a substrate, modern nano-scale FET structures, extensions of the various stochastic processes as well as a number of problems belonging to econophysics can be studied by the application of the semiconfined harmonic oscillator model [6–10]. For example, if the morphology, equilibrium crystal shape and shape evolution of a monocrystal of micron size grown on a substrate can be accurately predicted by the Gibbs–Curie–Wulff theorem [11], then one can assume that the exactly-solvable semiconfined model of the quantum harmonic oscillator can be considered as a good candidate for

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the accurate description of the above listed properties of the sub-micron or nano-sized crystallic structures grown on various substrates. A similar assumption is also true for the fabrication of advanced nano-scale QFETs which are considered as modern quantum well types of MOSFETs [12].

The main reason for the absence of such an oscillator model is due to the opinion that the semiconfined oscillator problem generalizing the non-relativistic oscillator in terms of the Hermite polynomials can not be solved exactly. In such problems, one is lead to approximate numerical solutions in terms of the zeros of Hermite functions [13]. Here, we show that such an exactly solvable model does exist provided one replaces the constant effective mass m_0 of the non-relativistic harmonic oscillator by a particular position-dependent effective mass $M(x)$.

The structure of the current paper is as follows: Section 2 collects some standard information about the non-relativistic quantum harmonic oscillator in the canonical approach, which energy spectrum $E_n \sim n+\frac{1}{2}$ and orthonormal wavefunctions of the stationary states expressed via the Hermite polynomials. Then, the model of the semiconfined quantum harmonic oscillator is presented in Section 3. There, we also propose the expression of the position-dependent effective mass for the model under study. We show that the corresponding Schrödinger equation has exact solutions with wavefunctions in terms of the generalized Laguerre polynomials, and that the energy spectrum for this model overlaps with the energy spectrum of the canonical non-relativistic quantum harmonic oscillator. Further discussion of the obtained results, including the correct limit relations from the constructed semiconfined model to the standard Hermite oscillator, is provided in the last section.

2 The non-relativistic canonical quantum harmonic oscillator

The non-relativistic quantum harmonic oscillator in the canonical approach is one of the most inspiring examples of exactly solvable quantum systems. Its beauty stems from the simplicity of the equidistant energy spectrum and the exact solution of the wavefunctions of the stationary states in terms of the Hermite polynomials. For further reference and for comparison with the new model, we are going to list some known results of this oscillator.

The one-dimensional time-independent Schrödinger equation for a non-relativistic quantum system reads

$$\hat{H}\psi(x) = E\psi(x), \tag{1}$$

where $\hat{H}$ consist of a kinetic and potential term

$$\hat{H} = \hat{H}_0 + V(x), \tag{2}$$

with

$$\hat{H}_0 = \frac{\hat{p}_x^2}{2m_0}. \tag{3}$$

Here, m_0 is a constant effective mass of the quantum system and in the canonical approach the momentum operator $\hat{p}_x$ is represented as

$$\hat{p}_x = -i\hbar\frac{d}{dx}. \tag{4}$$

For the quantum harmonic oscillator, the potential is given by

$$V(x) = \frac{m_0\omega^2x^2}{2}, \quad -\infty < x < +\infty, \tag{5}$$

where ω is a constant angular frequency. Substitution of (4) and (5) in the previous equations leads to the following second order differential equation:

$$\frac{\hbar^2}{2m_0}\frac{d^2\psi}{dx^2} + \left(E - \frac{m_0\omega^2x^2}{2}\right)\psi = 0. \tag{6}$$

The condition that $\psi(x)$ should tend to 0 when $x \to \pm\infty$ leads to the discrete energy spectrum $E \equiv E_n$ and the well known wavefunctions $\psi(x) \equiv \psi_n(x)$ [2]:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \ldots. \tag{7}$$

$$\psi_n(x) = e^{-\frac{m_0\omega}{2\hbar}x^2} H_n\left(\sqrt{\frac{m_0\omega}{\hbar}}x\right). \tag{8}$$

Herein, $H_n(x)$ is a Hermite polynomial, defined in terms of the ${}_2F_0$ hypergeometric function as follows [14]:

$$H_n(x) = (2x)^n \, {}_2F_0 \left(\begin{matrix} -n/2, -(n-1)/2 \\ - \end{matrix} ; -\frac{1}{x^2} \right). \tag{9}$$

The orthogonality relation for Hermite polynomials on the whole interval $(-\infty, +\infty)$,

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2} H_m(x) H_n(x) dx = 2^n n! \delta_{mn} \tag{10}$$

yields the following orthonormal wavefunctions $\tilde{\psi}_n(x)$:

$$\tilde{\psi}_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m_0 \omega}{\pi \hbar} \right)^{\frac{1}{4}} e^{-\frac{m_0 \omega x^2}{2\hbar}} H_n \left(\sqrt{\frac{m_0 \omega}{\hbar}} x \right). \tag{11}$$

3 Semiconfined harmonic oscillator model with a position-dependent effective mass

As announced in the Introduction, we are going to construct a non-relativistic quantum harmonic oscillator in the canonical approach, but with a different behavior of the wavefunctions than the "Hermite oscillator" of the previous section. Whereas the Hermite oscillator wavefunctions tend to zero at infinity, the wavefunctions of the oscillator model under construction tend to zero at the right side at $+\infty$, but from the left side already at some finite value of the position x, i.e. $\psi(x) = 0$ for $-\infty < x \leq -a$ with a a positive constant ($a > 0$). Therefore, we call the model a semiconfined harmonic oscillator. The vanishing of the wavefunctions of the oscillator model for $x \leq a$ implies that the potential $V(x)|_{x=-a}$ should tend to $+\infty$. One of the ways to achieve such an effect of an "infinite high wall" for the potential is to replace the constant effective mass m_0 of the oscillator system by a position-dependent effective mass $M(x)$.

The idea of an effective mass depending on the position is not new in physics. Its birth can be traced to the seminal experiment on the observation of tunneling of electrons in superconductors [15, 16]. A theoretical explanation of this effect was based on the assumption that the band structure changes with position within the independent-particle model of the superconductor [17]. Later, this assumption developed to the more general assumption stating that change of the band structure also changes an effective mass of the solid state system, and the following Hermitian version of the kinetic energy operator with position-dependent effective mass was proposed (it is also called as BenDaniel-Duke kinetic energy operator) [18]:

$$\hat{H}_0^{BD} = -\frac{\hbar^2}{2} \frac{d}{dx} \frac{1}{M(x)} \frac{d}{dx}. \tag{12}$$

Various modified versions of the BenDaniel-Duke kinetic energy operator have been introduced, based on different properties of the solid state structures [19–21]. However, it is shown that singular terms appearing in modified versions of the kinetic energy operator (12) and leading to a discontinuity of the wavefunction are compensated only in the case of the BenDaniel-Duke kinetic energy operator [22]. The Schrödinger equation with the BenDaniel-Duke kinetic energy operator (12) has been used successfully in a number of computations related to various aspects of non-relativistic quantum mechanics [23–26]. We have to note here that definition of Hermitian version of the kinetic energy operator with position-dependent effective mass via (12) and its modifications is not unique. Application of the contact point transformation method for the proper definition of the kinetic energy operator with position-dependent effective mass is proposed in [27] and it is also shown that such an application leads to a special case of the Von Roos kinetic energy operator [21] with $\alpha + \beta + \gamma = -1$, where $\alpha = -\frac{1}{4}$, $\beta = -\frac{1}{2}$ and $\gamma = -\frac{1}{4}$. More details of such interesting correspondence can be found in [28–30]. Another approach for generalizing the kinetic energy operator in the case of position-dependent mass is the introduction of the non-Hermitian PT symmetric kinetic energy operator [31] in which the ordinary derivative is replaced by the q-derivative [32]. Successful application of such an approach for the description of various quantum systems with position-dependent effective mass can be found in [33–37]. Here, we are going to use the BenDaniel-Duke kinetic energy operator (12) for our current computations highlighting that both contact point transformation and non-Hermitian PT symmetric generalization methods for the kinetic energy operator can also lead to attractive results with slightly different behaviour of the semiconfined oscillator model.

From a mathematical viewpoint it is interesting to study the behavior of exact solutions for wavefunctions and energy spectra for certain analytical expression of $M(x)$. For a semiconfined harmonic oscillator model, the expression of the position-dependent effective mass $M(x)$ should satisfy the following main conditions:

- The harmonic oscillator potential should have infinite high wall at the position $x = -a$, or $V(x) = +\infty$ for $-\infty < x \leq a$;

– The position-dependent effective mass $M(x)$ should yield the constant effective mass m_0 for $x = 0$, and also under the limit $a \to \infty$;
– The Schrödinger equation corresponding to the Hamiltonian with the BenDaniel-Duke kinetic energy operator and harmonic oscillator potential with the position-dependent effective mass $M(x)$ should be exactly solvable, i.e. with analytic expressions for the wavefunctions of the stationary states and for the energy spectrum;
– The obtained analytic expressions for the energy spectrum and the wavefunctions should reduce to (7) and (11) under the limit $a \to \infty$.

We propose the following simple analytic expression for the position-dependent effective mass $M(x)$:

$$M(x) = \begin{cases} \dfrac{am_0}{a+x}, & \text{for } -a < x < +\infty \\ +\infty, & \text{for } x \le -a \end{cases} \qquad (a > 0). \tag{13}$$

Note that this expression is different from certain standard choices for the mass function [33–35], but is chosen so as to serve for our purpose. It can indeed be verified that the conditions listed above are satisfied. First of all, one needs to rewrite the harmonic oscillator potential $V(x)$ via modification of (5) under the replacement $m_0 \to M(x)$:

$$V(x) = \frac{M(x)\,\omega^2 x^2}{2}, \quad -a < x < +\infty. \tag{14}$$

Now, one can easily observe that

$$V(-a) = +\infty. \tag{15}$$

Note that

$$\lim_{x \to +\infty} V(x) = +\infty.$$

Such a behavior of the harmonic oscillator potential implies the vanishing property of the wavefunction at $+\infty$.

Next, we easily observe from (13) that the second condition is satisfied:

$$M(0) = m_0 \quad \text{and} \quad \lim_{a \to \infty} M(x) = m_0. \tag{16}$$

Now we want to show that the Schrödinger equation corresponding to the Hamiltonian with the BenDaniel-Duke kinetic energy operator and harmonic oscillator potential with the position-dependent effective mass $M(x)$ is exactly solvable. Let us rewrite the Schrödinger equation corresponding to eqs. (12), (13) and (14):

$$\frac{d^2\psi}{dx^2} + \frac{1}{a+x}\frac{d\psi}{dx} - \frac{\frac{m_0^2\omega^2 a^2}{\hbar^2}x^2 - \frac{2m_0 aE}{\hbar^2}(a+x)}{(a+x)^2}\psi = 0. \tag{17}$$

Introduction of a new dimensionless variable $\xi = \frac{x}{a}$ gives

$$\frac{d^2\psi}{d\xi^2} + \frac{1}{1+\xi}\frac{d\psi}{d\xi} - \frac{\left(\lambda_0^4 a^4\right)\xi^2 - c_0\xi - c_0}{(1+\xi)^2}\psi = 0, \tag{18}$$

where

$$c_0 = \frac{2m_0 a^2 E}{\hbar^2}, \quad \lambda_0 = \sqrt{\frac{m_0\omega}{\hbar}}. \tag{19}$$

We look for exact solutions of eq.(18) of the following form

$$\psi = y(\xi)\,\varphi(\xi), \tag{20}$$

where $\varphi(\xi)$ is chosen as follows:

$$\varphi(\xi) = C \cdot (1+\xi)^A e^{B\xi}. \tag{21}$$

By substitution and performing straightforward computations, one can obtain that

$$A = \varepsilon_1\lambda_0^2 a^2, \quad B = \varepsilon_2\lambda_0^2 a^2, \quad \varepsilon_1 = \pm 1, \quad \varepsilon_2 = \pm 1, \tag{22}$$

and the second-order differential equation reduces to:

$$(1+\xi)\,y''(\xi) + \left[2(\varepsilon_1+\varepsilon_2)\lambda_0^2 a^2 + 1 + 2\varepsilon_2\lambda_0^2 a^2 \xi\right] y'(\xi) + \left[2(1+\varepsilon_1\varepsilon_2)\lambda_0^4 a^4 + \varepsilon_2\lambda_0^2 a^2 + c_0\right] y(\xi) = 0. \tag{23}$$

Now we need to take into account that our wavefunctions have to vanish at position values $\xi = -1$ ($x = -a$) and $\xi \to +\infty$ ($x \to +\infty$), in other words, the following limits must be satisfied:

$$\lim_{\xi \to +\infty} \varphi(\xi) = \lim_{\xi \to -1} \varphi(\xi) = 0.$$

Clearly, this only holds when A is positive and B negative. Thus only one of the four solutions of (22) remains:

$$\varphi(\xi) = C \cdot (1+\xi)^{\lambda_0^2 a^2} e^{-\lambda_0^2 a^2 \xi}. \tag{24}$$

Therefore, eq.(23) simplifies as follows:

$$(1+\xi) y''(\xi) + \left(1 - 2\lambda_0^2 a^2 \xi\right) y'(\xi) = \left(\lambda_0^2 a^2 - c_0\right) y(\xi). \tag{25}$$

This equation has polynomial solutions for y, by comparing it to the second order differential equation for the generalized Laguerre polynomials. Indeed, writing

$$\alpha = 2\lambda_0^2 a^2$$

in (25),

$$(1+\xi) y''(\xi) + (1 + \alpha - \alpha(1+\xi)) y'(\xi) = \left(\frac{\alpha}{2} - c_0\right) y(\xi), \tag{26}$$

one can see that a polynomial solution is given by

$$y_n(\xi) = L_n^{(\alpha)}(\alpha(\xi+1)), \tag{27}$$

provided

$$\frac{\alpha}{2} - c_0 = -n\alpha \quad \Leftrightarrow \quad c_0 = (n + \frac{1}{2})\alpha = (n + \frac{1}{2}) 2\lambda_0^2 a^2. \tag{28}$$

Herein, $L_n^{(\alpha)}(z)$ is the classical generalized Laguerre polynomial, satisfying the second order differential equation [14]

$$z\, p''(z) + (\alpha + 1 - z)\, p'(z) + n\, p(z) = 0, \qquad p(z) = L_n^{(\alpha)}(z) \tag{29}$$

given explicitly in terms of the ${}_1F_1$ hypergeometric function as follows:

$$L_n^{(\alpha)}(z) = \frac{(\alpha+1)_n}{n!} \, {}_1F_1\left(\begin{matrix} -n \\ \alpha+1 \end{matrix}; z\right). \tag{30}$$

From comparison of (28) and (19) one obtains that energy spectrum of the model under construction completely overlaps with energy spectrum of the non-relativistic quantum harmonic oscillator (7), i.e.

$$E \equiv E_n = \hbar\omega \left(n + \frac{1}{2}\right). \tag{31}$$

Rewriting the solution (27) in terms of the original data, the wavefunctions of the stationary states are expressed in terms of the generalized Laguerre polynomials as follows:

$$\tilde{\psi}_n(x) = C_n \cdot \left(1 + \frac{x}{a}\right)^{\frac{m_0\omega}{\hbar} a^2} e^{-\frac{m_0\omega}{\hbar} a(x+a)} L_n^{\left(2\frac{m_0\omega}{\hbar} a^2\right)} \left(2\frac{m_0\omega}{\hbar} a(x+a)\right), \quad (-a < x < +\infty) \tag{32}$$

where C_n is an orthonormalization parameter. It is useful to extend the domain of $\tilde{\psi}$ by putting $\tilde{\psi}(x) = 0$ for $x \le -a$. From the orthogonality relations of generalized Laguerre polynomials, one obtains

$$\int_{-\infty}^{+\infty} \tilde{\psi}_m(x)\tilde{\psi}_n(x)\, dx = \int_{-a}^{+\infty} \tilde{\psi}_m(x)\tilde{\psi}_n(x)\, dx = \delta_{mn},$$

for the following orthonormalization parameter:

$$C_n = (-1)^n \left(2\frac{m_0\omega}{\hbar} a^2\right)^{\frac{m_0\omega}{\hbar} a^2 + \frac{1}{2}} \sqrt{\frac{n!}{a\Gamma\left(n + 2\frac{m_0\omega}{\hbar} a^2 + 1\right)}}. \tag{33}$$

The obtained analytic expressions of the energy spectrum (31) and the wavefunctions of the stationary states (32) show that the third condition is satisfied. In the next section we will discuss some properties of the solution, and its behavior under the limit $a \to \infty$.

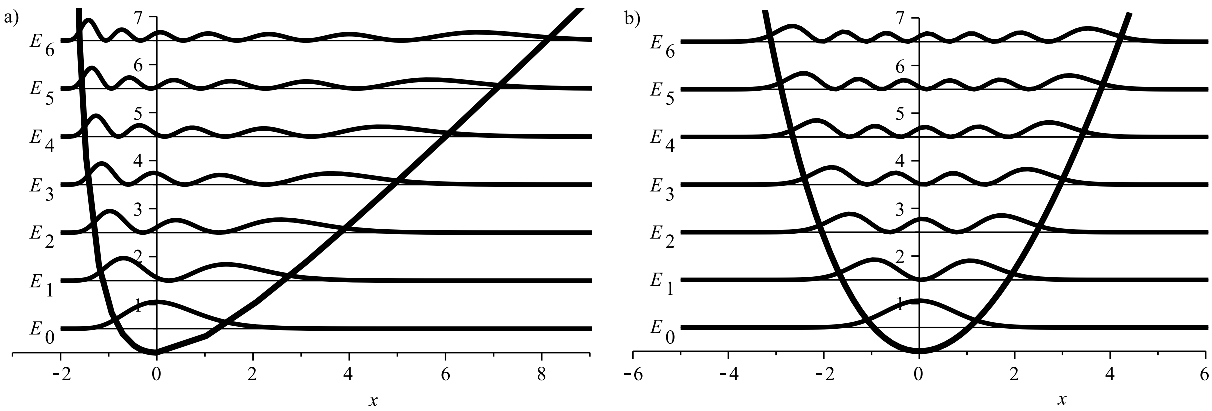

Fig. 1. The semiconfined quantum harmonic oscillator potential (14), the corresponding energy levels (31) and the probability densities $\left|\tilde{\psi}_n(x)\right|^2$ of the wavefunctions of the stationary states (32) for the ground and 6 excited states: a) for the confinement parameter $a = 2$; b) for the confinement parameter $a = 12$ ($m_0 = \omega = \hbar = 1$).

4 Discussion and Conclusion

Our main goal was to show that the Schrödinger equation corresponding to a Hamiltonian with the BenDaniel-Duke kinetic energy operator and a harmonic oscillator potential with position-dependent effective mass $M(x)$ of type (13) is exactly solvable. We obtained indeed orthonormalized wavefunctions of the stationary states (32) and the energy spectrum (31) of the semiconfined quantum system under study. It proves that our third condition is completely satisfied.

Let us now examine if our final condition is satisfied, i.e. if the obtained analytical expressions for the energy spectrum and for the wavefunctions reduce to the corresponding expressions (7) and (11) of the canonical non-relativistic quantum harmonic oscillator under the limit $a \to \infty$. For the energy spectrum, this is clear, as both spectra coincide. For the wavefunctions, it is useful to consider first some examples and some plots, in order to describe their behavior when a tends to infinity. In Figure 1, we present two such plots, for $a = 2$ and for $a = 12$. We plot here the potential function (14), the lowest energy levels E_n, and the probability densities $\left|\tilde{\psi}_n(x)\right|^2$, for $n = 0, 1, \ldots, 6$. One observes from the distribution of the probability densities that when the semiconfinement parameter a is close to zero, then the quantum system stays close to the infinitely high wall. As the value of the parameter a increases, the effect of the semiconfinement gradually disappears and the behavior becomes harmonic oscillator-like. This is a quite interesting phenomenon, and it shows the potential importance of this simple model.

The observation that the wavefunctions (32) tend to the Hermite oscillator wavefunctions (11) when $a \to +\infty$ can also be proved analytically. The actual computation is based on the following known limit relation between the Laguerre and Hermite polynomials [14]:

$$\lim_{\alpha \to +\infty} \left(\frac{2}{\alpha}\right)^{\frac{1}{2}n} L_n^{(\alpha)}\left((2\alpha)^{\frac{1}{2}} x + \alpha\right) = \frac{(-1)^n}{n!} H_n(x).$$

Therefore, one can check that the following limit holds:

$$\lim_{a \to +\infty} L_n^{\left(2\lambda_0^2 a^2\right)}\left(2\lambda_0^2 a (x+a)\right) = \frac{(-1)^n}{n!} H_n(\lambda_0 x).$$

Also, one can easily prove that

$$\lim_{a \to +\infty} \left(1 + \frac{x}{a}\right)^{\lambda_0^2 a^2} e^{-\lambda_0^2 a (x+a)} = e^{-\frac{\lambda_0^2 x^2}{2}}.$$

The reduction of the normalization parameter C_n under the limit $a \to +\infty$ is obtained using Stirling's approximation for the Gamma function. Thus the fourth condition is also satisfied: under this limit, the energy spectrum and the wavefunctions of the semiconfined oscillator model tend to those of the Hermite oscillator.

We consider the oscillator model introduced in this short paper as relevant. One the one hand, it is a very simple model which is exactly solvable, with an energy spectrum coinciding with the ordinary harmonic oscillator. On the other hand, it clearly exhibits a semiconfinement effect, for which no exactly solvable models existed so far. These properties can be important for the exploration of a number of physical phenomena in which semiconfinement appears. Unlike other known exactly-solvable harmonic oscillator-like models with a mass varying by position, this very simple model is still exactly solvable when it is under the action of an external homogeneous field $V_{ext} = gx$. In a forthcoming paper, we shall present these results, containing wavefunctions of the stationary states and energy spectrum of this extended model. Both the current oscillator model and the model under the external homogeneous field can be adopted further for the precise computation of the optical rectification, second-harmonic generation, electro-optic effect and other nonlinear optical properties of the semiconductor nanostructures of $GaAs/Al_xGa_{1-x}As$ type [38–40].

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