ON THE EXACT SOLUTION OF THE CONFINED POSITION-DEPENDENT MASS HARMONIC OSCILLATOR MODEL UNDER THE KINETIC ENERGY OPERATOR COMPATIBLE WITH GALILEAN INVARIANCE

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We propose exactly-solvable model of the confined harmonic oscillator in the framework of the effective mass formalism varying with position. Analytical expression of the position-dependent effective mass is chosen by such a way that it provides confinement effect for the via the infinitely high borders at value of position $x = \pm a$. Wave functions of the stationary states of the oscillator model under study have been obtained by solving exactly corresponding Schrödinger equation, which free Hamiltonian is compatible with Galilean invariance. Analytical expression of the wave function is described by the Gegenbauer polynomials, whereas obtained energy spectrum is discrete, but non-equidistant. It is shown that both energy spectrum and wave function completely recover known expressions of the so-called Hermite oscillator equidistant energy spectrum and wave function of the stationary states under the limit $a \to \infty$.

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1. INTRODUCTION

Quantum harmonic oscillator is one of the most attractive problems of the theoretical physics and pure mathematics [1,2]. Its attractiveness for theoretical physics is existence of the exact solutions in terms of the wave functions and energy spectrum of the quantum system under consideration in the framework of the various initial bounded conditions. Attractiveness of same quantum systems for pure mathematics is related with analytical expression of the wave functions, which are expressed through certain orthogonal polynomials of the Askey scheme. One needs to note that different orthogonal polynomials appear in the analytical expressions of the wave functions as a result of the initial conditions imposed to the quantum oscillator model. These initial conditions can be related with specific non-relativistic or relativistic behaviour of the oscillator model, but also the finite or infinite nature of the position that determines how the wave function is going to be bounded.

Non-relativistic quantum harmonic oscillator model with the wave functions bounded at infinity is well known [3]. Its energy spectrum is discrete and equidistant. Analytical expression of the wave function of this oscillator model with effective mass m_0 and angular frequency ω_0 is obtained through exact solution of the corresponding Schrödinger equation in terms of the Hermite polynomials. It is easy to observe that the wave function expressed via Hermite polynomials vanishs at $\pm\infty$. However, there is no any unique approach for the definition of the harmonic oscillator model with the wave function vanishing at finite region. One of the approaches is to look for approximate solutions of the Schrödinger equation describing non-relativistic quantum harmonic oscillator with the wave function bounded at finite region. Some examples of such approximate solutions having wide range applications from astrophysics to the nanotechnologies already exist [4-10]. Another approach, leading to exact solutions of similar oscillator model confined within the finite region is related with the replacement of the constant effective mass with the position-dependent effective mass formalism. Such a formalism was proposed within the theory explaining seminal experiment on the tunneling effect from superconductors within the free multi-particle approach with bandwidth changing with position [11]. Furthermore, the approach of the position-dependent effective mass has been successfully applied for explanation of the many experimental results and phenomena. Main goal of our paper is to develop this approach and apply it for exact solution of the non-relativistic quantum harmonic oscillator model with position-dependent effective mass with Galilean invariance.

The paper is structured as follows: Section 2 contains brief review of the well-known nonrelativistic quantum harmonic oscillator model, which wave functions of the stationary states are expressed through the Hermite polynomials. Then, we present main results devoted to the constructed model of the confined quantum harmonic oscillator possessing the position-dependent effective mass with Galilean invariance in Section 3. Final section is devoted to discussion of the obtained results. This section also includes basic limit relations between the model under construction and the so-called Hermite oscillator model.

2. NON-RELATIVISTIC HARMONIC OSCILLATOR IN TERMS OF THE HERMITE POLYNOMIALS

In this section, we are going to present general information about the problem of the non-relativistic quantum harmonic oscillator and its exact solution in

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terms of the wave functions of the stationary states and discrete energy spectrum. The information being provided in this section is well known and can be easily found in most of the textbooks devoted to quantum mechanics and its basic principles. However, we think that the information provided below can be useful for reader easily to understand the problem under consideration and its correct limits to the known harmonic oscillator results. First of all, one can start from the correct definition of the Schrödinger equation that in the position representation has the following form:

$$\left[\frac{\hat{p}_x^2}{2m} + V(x)\right]\psi(x) = E\psi(x). \quad (2.1)$$

Then, introducing exact expression of the quantum harmonic oscillator potential as

$$V(x) = \frac{m_0 {\omega_0}^2 x^2}{2}, \quad (2.2)$$

we can solve eq.(2.1) exactly assuming that eigenfunctions $\psi(x)$ of it vanish at infinity. Here m and ω_0 are position-independent mass and angular frequency of the non-relativistic quantum harmonic oscillator. We are going to perform all computation within the canonical approach to the quantum mechnics. Therefore, one-dimensional momentum operator is defined as below:

$$\hat{p}_x = -i\hbar\frac{d}{dx}. \quad (2.3)$$

Sustitution of both eqs.(2.2)&(2.3) at eq.(2.1) leads to the following second order differential equation:

$$\frac{d^2\psi}{dx^2} + \frac{2m_0}{\hbar^2}\left(E - \frac{m_0 {\omega_0}^2 x^2}{2}\right)\psi = 0. \quad (2.4)$$

Its exact solution in terms of the eigenvalues and eigenfunctions is well known. Energy spectrum E being as eigenvalue of eq.(2.4) is discrete and equidistant as follows:

$$E \equiv E_n = \hbar\omega_0\left(n + \frac{1}{2}\right), n = 0,1,\cdots. \quad (2.5)$$

Wave functions of the stationary states being as eigenfunctions eq.(2.4) have the following analytical expression:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega_0 x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega_0}{\hbar}}x\right). \quad (2.6)$$

Here, $H_n(x)$ are the Hermite polinomials. They are defined in terms of ${}_2F_0$ confluent hypergeometric functions [12]:

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

Wave functions (2.6) are ortonormalized in the whole real position range $(-\infty, +\infty)$:

$$\int_{-\infty}^{\infty} \psi_m^*(x)\psi_n(x)dx = \delta_{mn}.$$

This relation has been obtained via the following known orthogonality relation of Hermite polinomials $H_n(x)$:

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

3. EXACT SOLUTION OF THE CONFINED POSITION-DEPENDENT MASS HARMONIC OSCILLATOR MODEL IN TERMS OF THE GEGENBAUER POLYNOMIALS

This section deals with exact solution of the quantum harmonic oscillator problem confined in the finite region, which effective mass behaves itself as varying with position and being compatible with Galilean invariance. Beauty of such alternative method for description of the effective mass formalism within the non-relativistic quantum problem is the certain position dependency function that can also generate confinement effect as a hidden property of the model under consideration.

One of the approaches taking into account the mass varying with position in the kinetic energy operator is the approach that allows to introduce the following analytical expression of the kinetic energy operator compatible with Galilean invariance [13]:

$$\hat{H}_0^{GI} = -\frac{\hbar^2}{6}\left[\frac{1}{M(x)}\frac{d^2}{dx^2} + \frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx} + \frac{d^2}{dx^2}\frac{1}{M(x)}\right]. \quad (3.1)$$

Here, $M(x)$ is the effective mass varying with position. If one introduces confined harmonic oscillator potential as

$$V(x) = \begin{cases} \frac{M(x)\omega^2 x^2}{2}, & |x| < a, \\ \infty, & |x| \geq a. \end{cases} \quad (3.2)$$

then, the Hamiltonian describing the quantum harmonic oscillator problem confined in the finite region will have the following expression:

$$\hat{H}^{GI} = -\frac{\hbar^2}{6}\left[\frac{1}{M(x)}\frac{d^2}{dx^2} + \frac{d}{dx}\frac{1}{M(x)}\frac{d}{dx} + \frac{d^2}{dx^2}\frac{1}{M(x)}\right] + \frac{M(x){\omega_0}^2 x^2}{2}. \quad (3.3)$$

Performing easy computations one observes that (3.3) can be simplified as follows:

$$\hat{H}^{GI} = -\frac{\hbar^2}{2M}\left[\frac{d^2}{dx^2} - \frac{M'}{M}\frac{d}{dx} - \frac{1}{3}\frac{M''}{M} + \frac{2}{3}\left(\frac{M'}{M}\right)^2\right] + \frac{M(x){\omega_0}^2 x^2}{2}. \quad (3.4)$$

Position-dependent effective mass $M \equiv M(x)$ is only the function that is still indefinite in eq.(3.4). It can be defined within the following conditions:

- position-dependent effective mass $M(x)$ equals to constant mass m_0 at origin of position $x = 0$ and also recovers it under the limit $a \to \infty$;
- confinement effect at values of position $x = \pm a$ is achieved via the definition of the position-dependent effective mass $M(x)$;
- stationary Schrödinqer equation for the Hamiltonian $\hat{H}^{GI}$ (3.4) becomes exactly solvable and analytical solutions correctly recover Hermite oscillator solutions (2.5) & (2.6) under the limit $a \to \infty$.

We define position-dependent effective mass $M(x)$ satisfying the listed above conditions via the following analytical expression:

$$M \equiv M(x) = \frac{a^2 m_0}{a^2 - x^2}. \qquad (3.5)$$

Checking listed above conditions for the position-dependent effective mass $M(x)$ (3.5), one observes that it equals to constant mass m_0 under condition $M(0) = m_0$ and also recovers constant mass m_0 under the following limit relation:

$$\lim_{a\to\infty} \frac{a^2 m_0}{a^2 - x^2} = m_0. \qquad (3.6)$$

Aslo, one observes that potential (3.2) with position-dependent effective mass $M(x)$ (3.5) satisfies the following boundary conditions:

$$V(-a) = V(a) = \infty.$$

The final condition that one needs to check is exact solubility of the following Schrödinger equation with the Hamiltonian (3.4):

$$\hat{H}^{GI}\psi^{GI} = E^{GI}\psi^{GI}. \qquad (3.7)$$

By substitution of (3.4)&(3.5) at (3.7) and performing easy mathematical computations, one can write down the Schrödinger equation as follows:

$$\frac{d^2\psi^{GI}}{dx^2} - \frac{2x}{a^2 - x^2}\frac{d\psi^{GI}}{dx} + \frac{\left(\frac{2m_0 a^2 E^{GI}}{\hbar^2} - \frac{2}{3}\right)(a^2 - x^2) - \frac{m_0^2\omega_0^2 a^4}{\hbar^2}x^2}{(a^2 - x^2)^2}\psi^{GI} = 0. \qquad (3.8)$$

Now, one introduces new dimensionless variable $\xi = x/a$, which allows to rewrite eq.(3.8) in more compact form

$$\psi'' + \frac{\tilde{\tau}}{\sigma}\psi' + \frac{\tilde{\sigma}}{\sigma^2}\psi = 0. \qquad (3.9)$$

Here, $\psi \equiv \psi^{GI}$, $\tilde{\tau}$ is a polynomial of at most first degree, but σ and $\tilde{\sigma}$ are polynomials of at most second degree having the following mathematical expression:

$$\tilde{\tau} = -2\xi,\ \sigma = 1 - \xi^2,\ \tilde{\sigma} = \left(c_0 - \frac{2}{3}\right) - \left(c_2 - \frac{2}{3}\right)\xi^2,$$
$$c_0 = \frac{2m_0 a^2 E^{GI}}{\hbar^2},\ c_2 = c_0 + \frac{m_0^2\omega_0^2 a^4}{\hbar^2}.$$

Eq.(3.9) is exactly soluble second order differential equation of the hypergeometric type. There are various methods for its exact solution. One of such methods, which can be applied here is Nikiforov-Uvarov method for solution of the second order differential equations [14].

We assume that the wave function of the Schrödinger equation (3.9) has the following form:

$$\psi = \varphi(\xi)y(\xi), \qquad (3.10)$$

where, $\varphi(\xi)$ is defined as

$$\varphi(\xi) = e^{\int \frac{\pi(\xi)}{\sigma(\xi)}d\xi}, \qquad (3.11)$$

with $\pi(\xi)$ being at most a polynomial of first order. Also, by performing simple computations, one can show that

$$\psi' = \varphi y' + \frac{\pi}{\sigma}\varphi y,$$
$$\psi'' = \varphi y'' + \frac{2\pi}{\sigma}\varphi y' + \frac{\pi'\sigma - \pi\sigma + \pi^2}{\sigma^2}\varphi y.$$

Their substitution at eq.(3.9) leads to the following equation for $y(\xi)$:

$$y'' + \frac{2\pi + \tilde{\tau}}{\sigma}y' + \frac{\tilde{\sigma} + \pi^2 + \pi(\tilde{\tau} - \sigma') + \pi'\sigma}{\sigma^2}y = 0. \qquad (3.12)$$

One can easily check that $\tilde{\tau} - \sigma' = 0$. Then, by introducing

$$\bar{\tau} = 2\pi + \tilde{\tau}$$

and

$$\bar{\sigma} = \tilde{\sigma} + \pi^2 + \pi'\sigma,$$

eq.(3.12) can be written in more compact form as follows:

$$y'' + \frac{\bar{\tau}}{\sigma}y' + \frac{\bar{\sigma}}{\sigma^2}y = 0. \qquad (3.13)$$

Next, taking into account that $\bar{\sigma}$ is also a polynomial of at most second order, one can assume that $\bar{\sigma} = \lambda\sigma$. Then, we can rewrite (3.13) in the following more compact form:

$$y'' + \frac{\bar{\tau}}{\sigma}y' + \frac{\lambda}{\sigma}y = 0. \qquad (3.14)$$

At same time, one observes that

$$\pi = \varepsilon\sqrt{\mu\sigma - \tilde{\sigma}} = \varepsilon\sqrt{\left(\mu + \frac{2}{3} - c_0\right) - \left(\mu + \frac{2}{3} - c_2\right)\tilde{\sigma}},$$

where, $\mu = \lambda - \pi'$ and $\varepsilon = \pm 1$. Now, taking into account that π should be a polynomial at most of first degree, one observes that this condition is true if $\mu + \frac{2}{3} = c_0$ or $\mu + \frac{2}{3} = c_2$. Then, it means that we have four different solutions for π in terms of (ε, μ) pairs: $\left(+1, c_0 - \frac{2}{3}\right)$, $\left(+1, c_2 - \frac{2}{3}\right)$, $\left(-1, c_0 - \frac{2}{3}\right)$ and $\left(-1, c_2 - \frac{2}{3}\right)$. By computing exact expression of $\varphi(\xi)$, one can find that only at the value $\left(+1, c_0 - \frac{2}{3}\right)$, the wave function vanishes at $\xi = \pm 1$ $(x = \pm a)$. Then, one easily obtains that

$$\pi(\xi) = -\frac{m_0\omega_0 a^2}{\hbar}\xi,$$
$$\lambda = \frac{2m_0 a^2 E^{GI}}{\hbar^2} - \frac{m_0\omega_0 a^2}{\hbar} - \frac{2}{3},$$
$$\varphi(\xi) = (1 - \xi^2)^{\frac{m_0\omega_0 a^2}{2\hbar}}.$$

Taking into account that λ is known, then eq.(3.14) can be solved exactly through its comparison with the following second order differential equation for the Gegenbauer polynomials $C_n^{\bar{\lambda}}(x)$:

$$(1 - x^2)\bar{y}'' - (2\bar{\lambda} + 1)x\bar{y} + n(n + 2\bar{\lambda})\bar{y} = 0, \qquad (3.15)$$
$$\bar{y} = C_n^{\bar{\lambda}}(x).$$

From this comparison one obtains that energy spectrum E_n^{GI} is non-equidistant and has the following expression:

$$E_n^{GI} = \hbar\omega_0\left(n + \frac{1}{2}\right) + \frac{\hbar^2}{2m_0 a^2}n(n+1) + \frac{\hbar^2}{3m_0 a^2}. \qquad (3.16)$$

The wave functions of the stationary states ψ^{GI} expressed through the Gegenbauer polynomials by the following manner:

$$\tilde{\psi}^{GI}(x) = c_n^{GI}\left(1 - \frac{x^2}{a^2}\right)^{\frac{m_0\omega_0 a^2}{2\hbar}} C_n^{\left(\frac{m_0\omega_0 a^2}{\hbar} + \frac{1}{2}\right)}\left(\frac{x}{a}\right). \qquad (3.17)$$

Here, Gegenbauer polynomials $C_n^{\bar{\lambda}}(x)$ are defined in terms of the ${}_2F_1$ hypergeometric functions as follows [12]:

$$C_n^{(\bar{\lambda})}(x) = \frac{(2\bar{\lambda})_n}{n!} \quad {}_2F_1\left(\begin{matrix}-n, n+2\bar{\lambda} \\ \bar{\lambda}+\frac{1}{2}\end{matrix}; \ \frac{1-x}{2}\right), \bar{\lambda} \neq 0.$$

$\tilde{\psi}^{GI}$ is orthonormalized and differs from ψ^{GI} due to multiplied normalization factor c_n^{GI}, which is obtained from the following orthogonality relation for the Gegenbauer polynomials:

$$\int_{-1}^{1}(1-x^2)^{\bar{\lambda}-\frac{1}{2}} C_m^{(\bar{\lambda})}(x) C_n^{(\bar{\lambda})}(x)dx = \frac{\pi\Gamma(n+2\bar{\lambda})2^{1-2\bar{\lambda}}}{\{\Gamma(\bar{\lambda})\}^2(n+\bar{\lambda})n!}\delta_{mn}.$$

Its exact expression is the following:

$$c_n^{GI} = 2^{\frac{m_0\omega_0 a^2}{\hbar}}\Gamma\left(\frac{m_0\omega_0 a^2}{\hbar}+\frac{1}{2}\right)\sqrt{\frac{\left(n+\frac{m_0\omega_0 a^2}{\hbar}+\frac{1}{2}\right)n!}{\pi a\Gamma\left(n+\frac{2m_0\omega_0 a^2}{\hbar}+1\right)}}.$$

Taking into account that exact expressions of the energy spectrum and wave functions of the stationary states are found by solving the Schrödinger equation (3.7), this statement partly proves the final condition that introduced position-dependent effective mass $M(x)$ (3.5) needed to satisfy. We are going to discuss different properties and possible limit relations of these exact expressions within next Section.

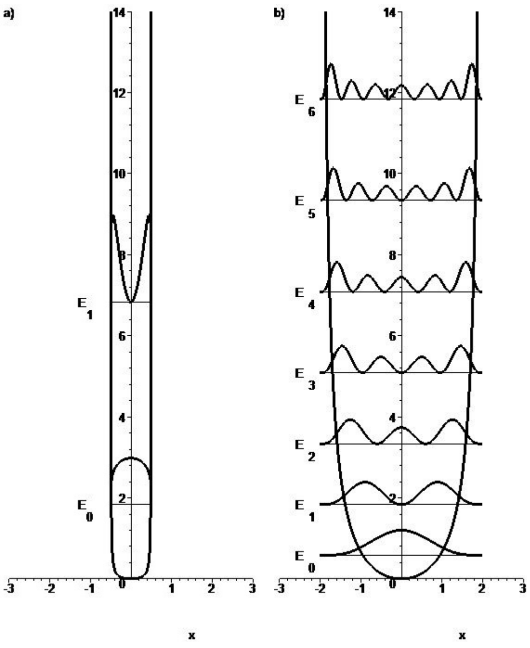

Fig. 1. Confined quantum harmonic oscillator potential (3.3) and behaviour of the corresponding non-equidistant energy levels (3.16) and probability densities $\left|\tilde{\boldsymbol{\psi}}^{GI}(\boldsymbol{x})\right|^2$ of the ground and a) **1** excited state for value of the confinement parameter $\boldsymbol{a} = \mathbf{0.5}$; b) **6** excited state for value of the confinement parameter $\boldsymbol{a} = \mathbf{2}$ ($\boldsymbol{m_0} = \boldsymbol{\omega_0} = \hbar = \mathbf{1}$).

4. DISCUSSION AND CONCLUSIONS

Taking into account that our main goal aiming to solve exactly the confined quantum harmonic oscillator model with position-dependent effective mass and kinetic energy operator compatible with Galilean invariance and show that obtained exact solutions under certain limit recover well-known Hermite oscillator model is achieved partially, namely, exact solution in terms of the wave functions of the stationary states and discrete energy spectrum are obtained, now one needs to explore further the possible limit from vanishing at finite region to infinite one. Confinement parameter a in fact restricts our oscillator model within the deep potential well with a width that equals to $2a$. Then, possible limit that one needs to apply here to expression of the discrete non-equidistant energy spectrum (3.16) and wave functions in terms of the Gegenbauer poynomials (3.17) is $a \to \infty$.

In Fig.1, we depicted both confined harmonic oscillator potential (3.2) with energy spectrum (3.16) and probability densities $\left|\tilde{\psi}^{GI}(x)\right|^2$ computed from the wave functions (3.17) and corresponding to energy spectrum (3.16). Two different values of the confinement parameter a is considered as an example - $a = 0.5; 2.0$. One observes from these two pictures that confinement parameter close to zero drastically changes the behaviour of the model under consideration from the quantum harmonic oscillator to infinite quantum well. Then of course, the question arises on mathematical base of such a behaviour.

Mathematical base of the correct recover of the known Hermite oscillator model is based on the following asymptotics and limit relations:

$$\underset{z\to\infty}{\Gamma(z)} \cong \sqrt{\frac{2\pi}{z}}e^{z\ln z - z},$$

$$\underset{\alpha\to\infty}{\Gamma(\alpha+1/2)} \cong \sqrt{2\pi}e^{\alpha\ln\alpha-\alpha}, \ \alpha = \frac{m_0\omega_0 a^2}{\hbar},$$

$$\lim_{a\to\infty}\Gamma(n+2\alpha+1) \cong 2^n\sqrt{4\pi\alpha}e^{(2\alpha+n)\ln\alpha-2\alpha+2\alpha\ln 2},$$

$$\lim_{a\to\infty}\alpha^{\frac{n}{2}}c_n^{GI} = \tilde{c}_0\sqrt{\frac{n!}{2^n}}, \quad \tilde{c}_0 = \left(\frac{m_0\omega_0}{\pi\hbar}\right)^{1/4}.$$

$$\lim_{a\to\infty}\left(1-\frac{x^2}{a^2}\right)^{\frac{1}{2}\sqrt{\alpha^2+1}} = e^{-\frac{m_0\omega_0 x^2}{2\hbar}}.$$

By applying these relations, one can easily to show the correctness of the following limit relation:

$$\lim_{a\to\infty}\psi_n^{GI}(x) = \psi_n(x).$$

This limit relation completes the proof of the correctness of the final condition for the position-dependent effective mass $M(x)$.

We do not discuss more details of the model that is presented in this paper, but at conclusions it is necessary to highlight an importance of such models due to recent development mothods, allowing to fabricate infinite quantum well structures with shapes different than traditional square-like behaviours.

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