International Journal of Applied Engineering Research ISSN 0973-4562 Volume 13, Number 12 (2018) pp. 10372-10375

Evolution of Thermal Expansion due to Anharmonic Potential

Adnan Jaradat[a*], Abdalla Obeidat[a], Maen Gharaibeh[a], Khaled Aledealat[a], Khitam Khasawinah[b], Mohammad Qaseer[a], Akram A. Rousan[a]

[a] *Physics Department, Jordan University of Science and Technology, Irbid, Jordan.*
[b] *Physics Department, Yarmouk University, Irbid, Jordan.*

[*] *Corresponding author*

Abstract

We demonstrate in this work the effect of an evolved anharmonic potential on the behavior of harmonic oscillator. We show that linear expansion starts to evolve as a result of the evolution of the potential. The effect on both the wave function and energy is also demonstrated.

Keywords: Fractional calculus; Anharmonic oscillator; Runge-Kutta method

INTRODUCTION

In a previous article [1] we studied the effect of an evolved electric potential on a charged particle placed in a harmonic oscillator and noted that the anharmonic oscillator will be studied fractionally to have a better understanding of thermal expansion. Thermal expansion is explained in solid state physics text books to be a phenomenon arises from the effect of an asymmetric term in the potential energy on the mean separation of a pair of atoms at a temperature T [2]. This term is proportional to x^3. We will introduce this term to the equation of the harmonic oscillator fractionally and observe the evolution of thermal expansion as the term develops from zero to its final form.

The problem of anharmonic oscillator was tackled by many researchers in the past. Abraham and Moses [3] obtained an exact solution by modifying the harmonic oscillator by introducing potentials in a predetermined way. Bender and Wu [4] considered an anharmonic oscillator having two terms of the orders x^2 and x^4 using the WKB technique to give some indication of the analytical structure of the more realistic field theory. Graffi et. al. [5] obtained better computational results by performing analytical continuation to Borel summability method. Singh et. al [6] used the theory of continued fractions to study the anharmonic oscillator containing terms of the order of x^2, x^4 and x^6 by writing the Green's function of the theory to prove that the continued fraction converges where the corresponding perturbation series in the dominant coupling diverges. Johnson III. et al [7] applied the variational method to determine the ground and first excited state energies of quartic and sextic anharmonic oscillator potentials. Starting from two sets of trial wave functions, they showed that by introducing additional terms, the energy eigenvalues gradually converge to those obtained from the Runge-Kutta numerical integration method. Also Koch et al [8] applied the variational method to calculate the first eight eigenvalues of quartic and sextic anharmonic oscillator potentials. By choosing a set of sophisticated trial wave functions, applying the orthogonal conditions between the eigenstates, and with the help of Maple software packages, they found that theses eight eigenvalues are accurate and agree well with those obtained from the Runge-Kutta numerical integration method. Floyd et al [9] introduced a quartic term αx^4 in the anharmonic oscillator. They found that , even though α, the coupling constant of the quartic term, can be very small, after large enough values of x the quartic potential αx^4 eventually supersedes the harmonic potential $m\omega x^2/2$, and it can no longer be considered weak. Li et al [10] studied the temperature dependence of the lattice dynamics of ScF_3 from 7 to 750 K. the measured phonon densities of states show a large anharmonic contribution with a thermal stiffening of modes around 25 meV. Amore [11] showed that it is possible to obtain numerical solutions to quantum mechanical problems involving a fractional Laplacian, using a collocation approach based on Little Sinc Functions (LSF), which discretizes the Schrödinger equation on a uniform grid. They applied this method collocation method to the fractional versions of the anharmonic oscillator and the Mathieu equation. In all mentioned works non used the idea of evolution in studying the anharmonic oscillator and thermal expansion except for the last reference [11] where the fractional Laplacian was used as an application of fractional calculus.

As mentioned in our previous work, fractional calculus in the sense of derivatives was not utilized, but the idea of evolution which is one of the outcomes of fractional calculus was reemployed in the present work by applying a developing potential which causes the phenomenon of thermal expansion. The idea of evolution of physical phenomena has been introduced and studied by many researchers. Engheta [12,13] applied the idea to the electromagnetic multipole showing the evolution of multipole from a certain order to the higher one. Gómez-Aguilar and co-workers contributed intensively to the field of fractional calculus. They studied fractional electrical circuits. They introduced an analytical solution to an RLC circuit in terms of the Mittag-Leffler function depending on the order of the fractional differential equation [14,15]. Also they studied the transitory response and analyzed time and frequency domain of RC circuit applying Caputo fractional derivative [16,17]. Moreover they described the dynamics of charged particles in electric fields employing Laplace transform of Caputo derivative [18]. They also used Fourier method to find the full analytical solution of electromagnetic wave in conducting media considering Dirichlet conditions [19]. Rousan et al [20] have studied such evolution in gravity and showed the evolution of a semi-infinite linear mass from a mass point. Rousan et al [21] showed how the oscillatory behavior (LC circuit) goes over a decay behavior (RC circuit) as the order of fractional differentiation goes from zero to one, and vice versa. Also Rousan et al [22] studied fractional harmonic oscillator and suggested that the system goes through an evolution process as the fractional order goes from zero (free) to one (damped), letting it pass through intermediate stages where the system can have a damping character and the material can be thought as a pseudo-damping material. Fractional electrical circuits were studied and analyzed from all aspects by Kaczorek and Rogowski [23,24]. Obeidat et al [25] studied the evolution of a current in a wire and estimated the time required for the current to reach its maximum value. Good bibliography on evolution process and fractional calculus can be found in [20-22] and [1, 25].

METHOD

The time independent Schrödinger equation in one dimension is given by:

$$-\frac{\hbar}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \qquad (1)$$

Where $\hbar$ is the normalized Blank constant, m is the mass of the particle under the influence of the potential energy $V(x)$, E is the energy of the system and ψ is the total wave function. One of the most important potentials in quantum mechanics which has an exact solution is the harmonic potential; $V=\frac{1}{2}m\omega^2x^2$, where ω is the frequency of the oscillator. Then the above equation reduces to:

$$\frac{d^2\psi(x)}{dx^2}=-\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2\right)\psi(x) \qquad (2)$$

This equation can be solved by means of applying Frobenius method [26] or by means of the Adomian decomposition method [27], and the final result is:

$$\psi(\xi)=H_n(\xi)e^{-\frac{\xi^2}{2}} \qquad (3)$$

Where $\xi=\left(\frac{m\omega}{\hbar}\right)^2x$ and $H_n(\xi)$ is the Hermite polynomial of order n. The energy of the system is:

$$E_n=\hbar\omega\left(n+\frac{1}{2}\right), \qquad n=0,1,2,.... \qquad (4)$$

Even though the harmonic theory explained many physical properties in physics, and open an elegant method of solving complicated problems through the second quantization, but it failed to predict thermal expansion due to the symmetry of the potential. Thermal expansion, μ, is proportional to the expectation value of the distance, x, i.e. $\mu\sim<x>$. Since the potential is symmetric, the wave function as shown in eq.3 is either even or odd function. The expectation value of x is given as:

$$<x>=\int_{-\infty}^{\infty}x\,|\psi(x)|^2\,dx \qquad (5)$$

Since the square of either an even function or an odd function is an even function, so the integrand is always an odd function and consequently, the value of the integration is zero. In general, to have a value for the expectation value of x, one has to distort the symmetry of the potential, this is doable by adding a non-symmetric term to the potential such as βx^3

In this work, we will study the effect of an evolving anharmonic term of the form:

$$-\alpha\beta x_0^{1-\alpha}x^{2+\alpha} \qquad (6)$$

Where α varies from 0 to 1 to be added to the oscillator, the time independent Schrödinger equation will read as:

$$\frac{d^2\psi(x)}{dx^2}=-\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2+\alpha\beta x_0^{1-\alpha}x^{2+\alpha}\right)\psi(x) \qquad (7)$$

Where the factor $x_0^{1-\alpha}$ is introduced to take care of units.

This extra term in this form will set a developing potential which in turn will be the source of thermal expansion.

The above equation has been solved numerically by following the method used in our previous work, i.e., the Numerov algorithm [1]. It was shown that this algorithm is simpler and produces higher accuracy than using the Runge-Kutta method, and it was also shown by others that the Numerov algorithm is faster and more stable [28,29].

Applying the Numerov method to the general form of the second order differential equation of the form:

$$\frac{d^2y(x)}{dx^2}=-g(x)y(x)+s(x) \qquad (8)$$

Where $g(x)$ and $s(x)$ are known functions, in our case these functions are given by:

$$g(x)=\frac{2m}{\hbar^2}\left(E-\frac{1}{2}m\omega^2x^2+\alpha\beta x_0^{1-\alpha}x^{2+\alpha}\right) \qquad (9)$$

And $s(x)=0$, with the following initial conditions: $y(x_0)=y_0$ and $y'(x_0)=y_0'$, the final form of the Numerov's formula is then:

$$y_{n+1}=\frac{(12-10f_n)y_n-f_{n-1}y_{n-1}}{f_{n+1}} \qquad (10)$$

With:

$$f_n=1+g_n\frac{(\Delta x)^2}{12} \qquad (11)$$

Where Δx is the step. A full derivation of Numerov algorithm can be found somewhere else [30]

In the present work, all the constants are taken to be equal to one except for the parameter β.

Figure 1 shows how the potential varies for different values of α at $\beta=0.05$ and how it varies with β at α=5/9. One has to be very careful of picking the values of β, since for relatively high value the extra term of the potential will be dominant for high values of x, and the general solution to the Schrödinger equation will be impossible to achieve even with the help of perturbation theory. In all results this parameter was chosen to be 0.01.

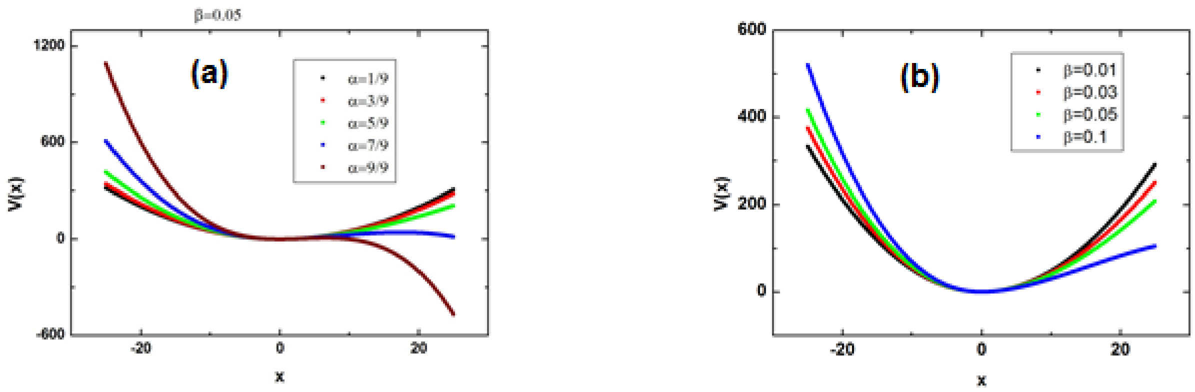

Figure 1. (a) The potential for β=0.05 with different values of α. **(b)** The potential for α=5/9 with different values of β.

RESULTS AND DISCUSSION

By introducing a developing term as a potential to Schrödinger equation representing the harmonic oscillator an asymmetry starts to show in the potential. It was shown in Figure 1 that care must be taken when assigning a numerical value of the parameter β, the suggested value was 0.01 for the reasons mentioned in the previous section.

The evolution of the potential is facilitated by increasing the value of the fractional term α. This term was increased in steps from zero to one. Figure 2 shows how the shape of the potential changes from a symmetrical shape when α=0 (α=0 coincides with α=1/9) to a full asymmetry when α=1. When the potential is symmetric the equilibrium separation between the neighboring atoms remains the same irrespective of the energy, which means that no thermal expansion can occur. When α deviates from zero asymmetry starts to show and the mean separation starts to increase with increasing energy. This figure makes clear how the asymmetry starts to evolve by increasing the "strength" of the new term via the value of β.

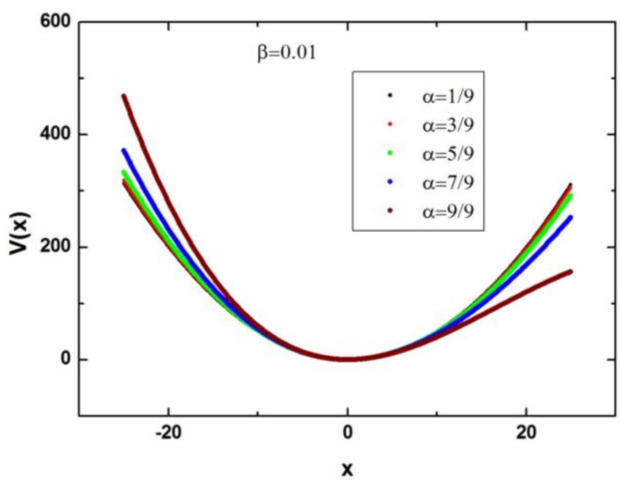

Figure 2. The potential for different values of α with β=0.01

The expectation value of x (i.e. thermal expansion) should increase with energy (temperature) and that is evident from the results shown in figure 3. In this figure the expectation value of x is plotted versus energy (n) for different values of α. It clear that as the value of α increases, which means that the asymmetry term becomes "stronger" the value of $< x >$ increases. Also, as expected the value of $< x >$ increases as the energy (n) increase.

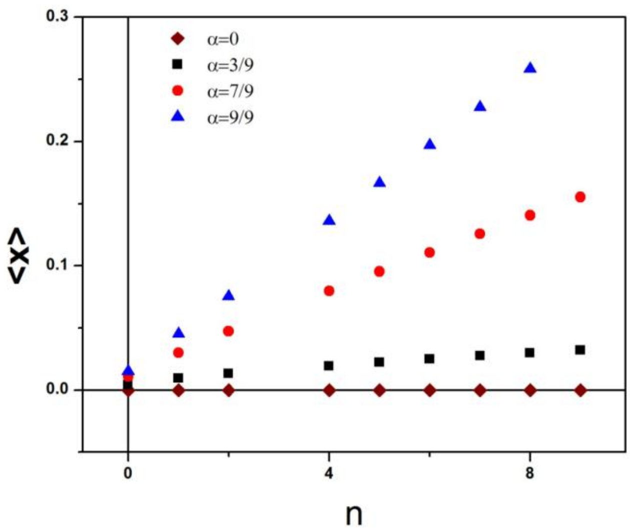

Figure 3. The expectation value of x with energy (n) for different values of α.

Finally Figure 4 shows the potential and the values for the expectation values of x (the equilibrium separation) are shown by the dotted line which indicates how $< x >$ increases with energy.

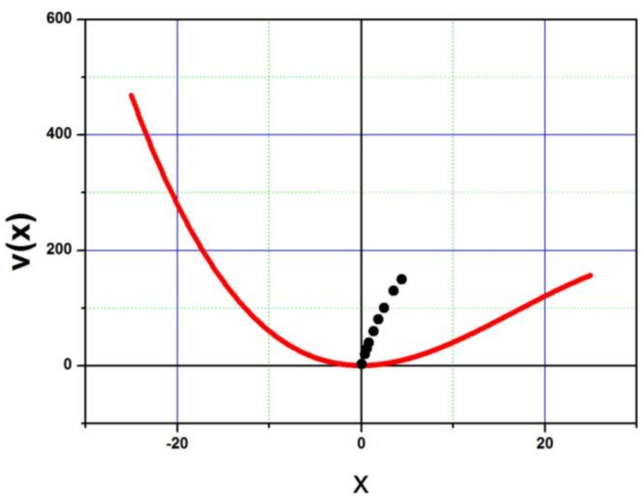

Figure 4. The potential energy with dotted line denoting the $< x >$ for different values of energy (n)

CONCLUSION

Anharmonic oscillator was developed by adding an asymmetrical potential fractionally to the harmonic oscillator. Asymmetry developed gradually with increasing the fraction gives rise to thermal expansion. It was demonstrated that the expansion increased with increasing the fraction of asymmetry and with increasing energy, as expected.

REFERENCES

[1] A. Jaradat, A. Obeidat, M. Gharaibeh, K. Aledealat, K. Khasawinah, M. Qaseer, and A. A. Rousan. *Revista Mexicana de F´ısica **63** (2017)*

[2] Charles Kittle, Introduction to Solid State Physics, 5th edition, John Wiley & Sons (1976) pp. 142.

[3] P. B. Abraham and Moses, Physical Review A, **22**(4), 1980

[4] Carl M. Bender and Tai Tsun Wu, The Physical Review, **184**(5), 1969

[5] S. Graffi, V. Gricchi and Simon. Physics Letters **32B**(7), 1970

[6] Vircndra Singh, S. N. Biswas and K. Datta. *Physical Review D. 18 (1978).*

[7] Thomas L. Johnson III, Elizabeth R. Hegdahl, Andrew R. Ward, and Stanley E. Schnell. *Journal of Undergraduate Research in Physics MS134 (2008).*

[8] Joshua M. Koch, Christopher F. J. Schuck, and Bronson W. Wacker. *Journal of Undergraduate Research in Physics MS134 (2008).*

[9] Benjamin T. Floyd, Amanda M. Ludes, Chia Moua, Allan A. Ostle, and Oren B. Varkony. *Journal of Undergraduate Research in Physics (2012).*

[10] Chen W. Li, Xiaoli Tang, J. A. Mun˜oz, J. B. Keith, S. J. Tracy, D. L. Abernathy, and B. Fultz. *PHYSICAL REVIEW LETTERS PRL 107, 195504 (2011).*

[11] Paolo Amore, Francisco M. Fern´andez *INIFTA*, Christoph P. Hofmann, and Ricardo A. S´aenz *Journal of Mathematical Physics · December 2009*

[12] N. Engheta, *IEEE Trans. Antennas Propag.* **44** (1996) 554.

[13] . N. Engheta, *Microw. Opt. Technol. Lett.* **23** (1999) 100.

[14] J.F. G´omez-Aguilar, *Rev. Mex. F´ıs.* **62** (2016) 144.

[15] J.F. G´omez-Aguilar, R. Razo-Hernandez, D. Granados-Lieberman, *Rev. Mex. F´ıs.* **60** (2014) 32-38.

[16] F. G´omez, J. Rosales, & M. Guia, *Central European Journal of Physics,* **11** (2013) 1361-1365.

[17] Guia, M., G´omez, F., & Rosales, *J. Open Physics*, **11** (2013) 1366-1371.

[18] J.F. G´omez-Aguila & E. Alvarado-M´endez, (2015) (pp. 147-158) Springer Netherlands.

[19] J.F. G´omez-Aguilar, H. Y´epez-Martinez, C. Calder´on-Ram´on,M. Benavidez-Cruz, & L.J. Morales-Mendoza, *Journal of Electromagnetic Waves and Applications* (2015) 1-13.

[20] A. Rousan, E. Malkawi, E. Rabei, H. Widyan, *Fract. Calc.Appl. Anal.* **5** (2002) 155.

[21] A. Rousan *et al. Fract. Calc. Appl. Anal.* **9** (2006) 33.

[22] A. Rousan N. Ayoub K. Khasawineh, *Int. J. Apllied Math.* **19** (2006) 263.

[23] T. Kaczorek, & K. Rogowski, Springer International Publishing. (2015) (pp. 81-115).

[24] T. Kaczorek, & K. Rogowski, (2015) Springer International Publishing (pp. 49-80).

[25] A. Obeidat, M. Gharaibeh, M. Al-Ali, A. Rousan, *Fract. Calc. Appl. Anal.* **14** (2011) 247.

[26] Gasiorowicz S. *Quantum physics*. Hoboken, NJ: Wiley. 336 pp. 3. ed., (2003)

[27] A. K. Jaradat, A. A. Obeidat, M. A. Gharaibeh, M. K. Hasan Qaseer.

[28] *International Journal of Applied Engineering Research.* **13**, 2 (2018) pp. 1056-1059.

[29] M.M. Chawla, *BIT Numerical Mathematics* **24** (1984) 117-8.

[30] C.P. Katti, K. Chopra, *International Journal of Computer Mathematics* (1990) 221-6.

[31] R. Gonsalves Phy410-505-2009. *Computational Physics*. https://www.physics.buffalo.edu/phy 410-505-2009/. (2009).