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Establishing mathematical models for determining quantum dot potential for pbs and pbte structures in terms of QD's diameters by numerical methods

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Abstract

The main goal of this paper is to obtain the estimated determination of the quantum dot potential for PbS and PbTe structures (in mV) which are compared to other values at different QD's diameters (in nm). In order to investigate this goal, the study relies on two methods of interpolation such as Neville and Spline methods, as well as it constructs mathematical models that help to find the estimate determination of quantum dot potential for PbS and PbTe structures compared to other values at different QD's diameters. The numerical results were very close to the real results. Finally, we estimated the determinations outside the fields and labs of the measured areas.

Keywords: Mathematical model, Neville's method, Spline method, Quantum dot potential for PbS and PbTe, Diameter.

1. Introduction

The solution of the physics problems has been considered one of the most interested topics in applications. Therefore, in this paper, we attempt to get the estimated determination of the quantum dot potential for PbS and PbTe structures (in mV) which are compared to other values at different QD's diameters (in nm). Moreover, even though there are many theoretical studies on combines between mathematics and physics problems. For examples, in 2016, Arif, G. E., et al., introduced

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the mathematical modeling to calculate uranium concentrations in the urine samples of the factory's workers due to the number of working years [4]. In 2016, Ammar A. Battawy, et, al., studied the measurement of interior radon concentration in different Iraqi radiation lands[5]. Furthermore, in 2016, Arif, G. E., and Al-Douri, Y., presented the mathematical modeling of physical properties for Hexagonal Binaries [3]. In 2017, through using Neville and Hermite methods Hameed, R. A., et, al., studied the estimating the amount of potassium radiation effect on soil [7]. In addition, in 2017, Arif, G. E., et, al., showed estimated the amount of uranium radiation effect on the workers in selected chemical factories relying on the numerical analysis spline method [2]. In 2019 Luma. N. M., et, al., numerical method has been applied to study estimate the rate of contamination in Baghdad soils, see [8]. The study depends on mathematical modeling process and utilizing numerical analysis methods to conduct the calculations of the (PbS) and the (PbTe). However, in this paper, the new mathematical models have been established through relying on Neville and spline methods to estimate the calculations and we try to understand the physics problems through solve the mathematical models numerically.

2. Neville's Method [6, 9]

In Lagrange interpolation there is a practical difficulty which is the difficulty of applying the error term, therefore, the required polynomial degree for the wanted accuracy is unknown if calculations are not conducted. A general procedure is to calculate the given results of different polynomials until the achievement of suitable agreement. Thus, the work achieved by the second polynomial in calculating the approximation does not reduce the required work for calculating the third approximation. In addition, it is also not easy to acquire the fourth approximation when the third approximation is known and so on. We can deduce these approximating Polynomials in away by employing previous calculations to a greater benefit.

Definition1: let f be a function defined at $x_0, x_1, x_2, \ldots, x_n$ and make $m_1, m_2, \ldots, m_k$ distinct integers, with $0 \leq m_i \leq n$ for each i the Lagrange polynomial that is in agreement with $f(x)$ at k points $xm_1, xm_2, \ldots, xm_k$ is signified $pm_1, pm_2, \ldots, pm_k$

Theorem 2.1. *Let f be defined at $x_0, x_1, x_2, \ldots, x_n$, and let x_j, x_i be two distinct numbers in this set. Then*

$$p(x) = \frac{(x - x_j)p_{0,1,\ldots,j-1,j+1,\ldots,k}(x) - (x - x_i)p_{0,1,\ldots,i-1,i+1,\ldots,k}(x)}{(x_i - x_j)} \tag{2.1}$$

is the $k-th$ Lagrange polynomial that interpolates f at the $k+1$ points $x_0, x_1, x_2, \ldots, x_k$.

Using the Nivelle's method to calculate the amount (PbTe). Since,

$$f(x_0) = 1.07 \qquad x_0 = 65$$
$$f(x_1) = 1.06 \qquad x_1 = 67$$
$$f(x) = \frac{(x - x_0)f(x_1) - (x - x_1)f(x_0)}{(x_1 - x_0)} = \frac{(x - 0.65)1.06 - (x - 67)1.07}{67 - 65} = -0.005x + 1.395$$

Table 1: The resulted values obtained by the mathematical model proposed to det. the quantum dot potential for PbTe structure (in mV) are compared to the exp. values, which are based on QD's diameter (in nm) [1].

NO.	***pbTe OD's Diameter***	***pODCal*** $\times 10^{-3} Exp.$	***pODCal*** $\times 10^{-3} Det.$	***Error***
1	***65***	***1.07***	***1.07***	***0***
2	***67***	***1.06***	***1.06***	***0***
3	***68***	***1.04***	***1.055***	***0.015***
4	***69***	***1.03***	***1.05***	***0.02***
5	***70***	***0.98***	***1.045***	***0.065***
6	***71***	***0.95***	***1.04***	***0.09***

Figure 1 shows the diagram between experimental and estimated values for (PbTe) by using the Nivelle's method.

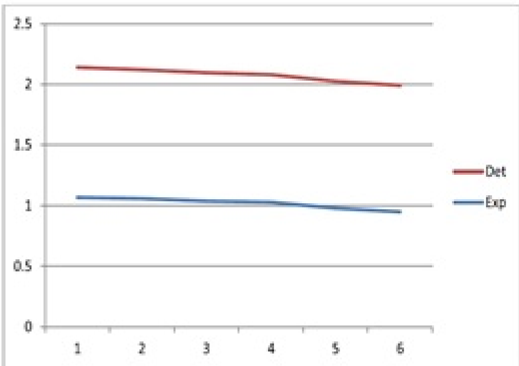

Figure 1: Diagram between exp. and estimated values for (PbTe) using the Nivelle's method.

Using the Nivelle's method to calculate the amount (PbS), then we have

$$f(x) = \frac{(x - x_0)f(x_1) - (x - x_1)f(x_0)}{(x_1 - x_0)}$$

since,

$$\begin{aligned} f(x_0) &= 1.36 \qquad x_0 = 60 \\ f(x_1) &= 1.35 \qquad x_1 = 61 \end{aligned}$$

then

$$f(x) = \frac{(x - 0.60)1.35 - (x - 61)1.36}{61 - 60} = -0.01x + 1.96$$

Table 2: The resulted values obtained by the mathematical model proposed to det. the quantum dot potential for PbS structure (in mV) are compared to the exp. values, which are based on QD's diameter (in nm) [1].

NO.	pbTe OD's Diameter	pODCal $\times 10^{-3} Exp.$	pODCal $\times 10^{-3} Det.$	Error
1	60	1.36	1.36	0
2	61	1.35	1.35	0
3	62	1.29	1.34	0.05
4	63	1.24	1.33	0.09
5	64	1.18	1.32	0.14
6	65	1.14	1.31	0.17

Figure 2 presents the diagram between experimental and estimated values for (PbS) by utilized the Nivelle's method.

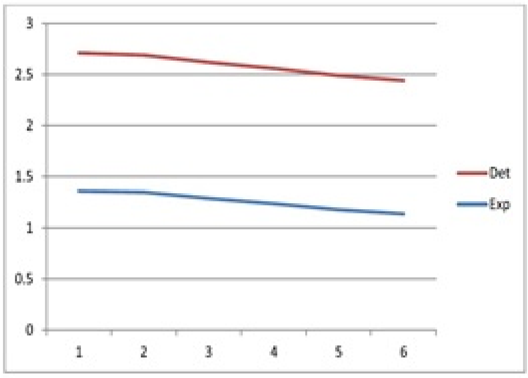

Figure 2: Diagram between exp. and estimated values for (PbTe) using the Nivelle's method.

3. Linear Spline [10]

let the given data point be (x_j, y_j) $a = x_0 < x_1 < x_2 < \cdots < x_n = b$, where $j = 1, 2, \ldots, n$, $h_i = x_i - x_{i-1}$, and let be the spline of degree one defined in the interval $[x_{j-1}, x_j]$. Further, let S_j obviously, $S_j(x)$ represents a straight line joining the points (x_{j-1}, y_{j-1}) and (x_j, y_j). Hence, we write.

$$\begin{aligned} S_j(x) &= y_{j-1} + m_j(x - x_{j-1}) \\ m &= \frac{y - y_{j-1}}{x - x_{j-1}} \end{aligned} \tag{3.1}$$

where, successively in (3.1). We obtain different spline of degree one valid in setting $j = 1, 2, \ldots, n$. The subintervals j to n respectively. It is easily seen that $S_j(x)$ continuous at both the end points. Using the spline method to calculate the amount (PbTe) as following:

$$f(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

since,

$$f(x_0) = 1.07 \qquad x_0 = 65$$
$$f(x_1) = 1.06 \qquad x_1 = 67.$$

Then

$$f(x) = 1.07 + \frac{-0.01}{2}(x - 65) = 1.395 - 0.005x$$

Table 3: The resulted values obtained by the mathematical model proposed to det. the quantum dot potential for PbS structure (in mV) are compared to the exp. values, which are based on QD's diameter (in nm) [1].

NO.	***pbTe OD's Diameter***	***pODCal*** $\times 10^{-3} Exp.$	***pODCal*** $\times 10^{-3} Det.$	***Error***
1	***65***	***1.07***	***1.07***	***0***
2	***67***	***1.06***	***1.06***	***0***
3	***68***	***1.04***	***1.055***	***0.015***
4	***69***	***1.03***	***1.05***	***0.02***
5	***70***	***0.98***	***1.045***	***0.065***
6	***71***	***0.95***	***1.04***	***0.09***

By using the spline method, Figure 3 presents the relation between experimental and estimated values for (PbS).

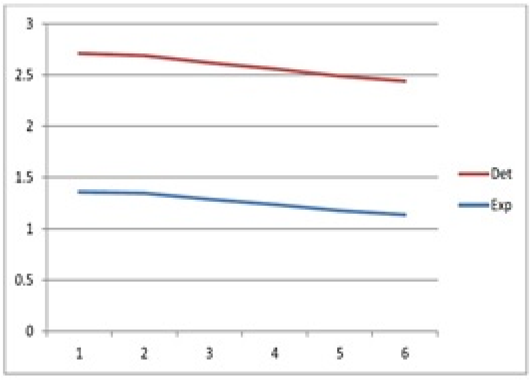

Figure 3: Diagram between exp. and estimated values for (PbTe) using the spline method.

To calculate the amount (PbS), we employed the spline method as following.

$$f(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0)$$

since,

$$f(x_0) = 1.36 \qquad x_0 = 60$$
$$f(x_1) = 1.35 \qquad x_1 = 61, \quad \text{then}$$
$$f(x) = 1.36 - 0.01(x - 60) = 1.96 - 0.01x$$

Table 4: The resulted values obtained by the mathematical model proposed to det. the quantum dot potential for PbS structure (in mV) are compared to the exp. values, which are based on QD's diameter (in nm) [1].

NO.	pbTe OD's Diameter	pODCal $\times 10^{-3}$ *Exp.*	pODCal $\times 10^{-3}$ *Det.*	Error
1	60	1.36	1.36	0
2	61	1.35	1.35	0
3	62	1.29	1.34	0.05
4	63	1.24	1.33	0.09
5	64	1.18	1.32	0.14
6	65	1.14	1.31	0.17

Figure 4 illustrates the relation between experimental and estimated values for (PbS) using the spline method.

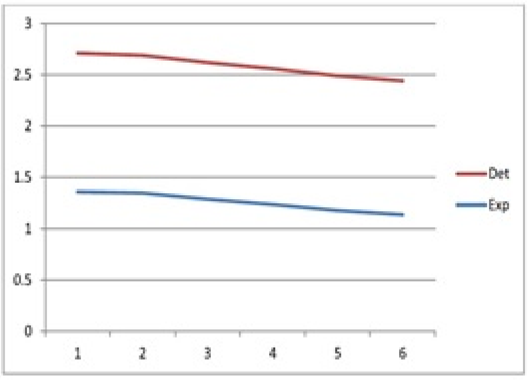

Figure 4: Diagram between exp. and estimated values for (PbS) using the spline method.

To comparing between the Nivelle and Spline methods, through the absolute error that obtaining from the two methods, we conclude that the Nivelle and Spline method are equivalent in computing sums of (PbTe) and (PbS), see Tables 5 and 6.

Table 5: Comparing the error ratio between the Nivelle and Spline methods for calculating the amount (PbTe).

NO.	Nivelle method	Spline method
1	0	0
2	0	0
3	0.015	0.015
4	0.02	0.02
5	0.065	0.065
6	0.09	0.09

Table 6: Comparing the error ratio between the Nivelle and Spline methods for calculating the amount (PbS).

NO.	***Nivelle method***	***Spline method***
1	***0***	***0***
2	***0***	***0***
3	***0.05***	***0.05***
4	***0.09***	***0.09***
5	***0.14***	***0.14***
6	***0.17***	***0.17***

4. Conclusions

The purpose of this study relies on two methods of interpolation such as Neville and Spline methods, as well as it constructs mathematical models that help to conclude the estimate determination of quantum dot potential for PbS and PbTe structures compared to other values at different QD's diameters (in nm). Finally, we realize that the numerical results were very close to the real results.

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