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Use of Spreadsheet for the Perturbation Theory in Quantum Harmonic Oscillator

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Abstract: The objective of this article is to graphically illustrate to the students the physical phenomenon of perturbation of quantum harmonic oscillator by simulating it on a computer using spreadsheets. Eigen functions in different states of the harmonic oscillator are obtained using interactive spreadsheet. Spreadsheets can be setup to solve numerical solutions of complex systems. This will make the concept, which so far is left to the abstract imagination come alive for the student and initiate a deeper understanding of particle motion.

Key words: Physics Education · Perturbation · Eigen functions · Spreadsheets · Harmonic oscillator

INTRODUCTION

Computer assisted education is more effective than traditional methods to learn science and technology principles [1, 2]. One opportunity offered by the use of computers is the ability to conduct simulations, which have become a powerful tool in university physics education. Spreadsheets can be a powerful pedagogical tool in physics teaching-learning. From data analysis and graphing to animation and simulations, Microsoft Excel® is a very versatile program for the teachers and students. The strong features of spreadsheet are their cell based structure and the simple interface that is easy to use for new users also. Excel is a powerful spreadsheet with VBA robust programming capabilities that can be a powerful tool for teaching physics concepts. The advantage of using a spreadsheet in teaching-learning process is that the programming is streamlined and less time is needed to enter the necessary code. In a spreadsheet, the data manipulations are held in front of the user in a very direct and accessible manner. In addition, the spreadsheet program itself provides for screen graphics, charts and easy-data manipulation using large number of functions, on-screen numerical and visual feedback and fast calculations [3-5]. Graphics and Charting capabilities enhance the effectiveness of spreadsheets as a learning tool by providing visual images that enable students to observe the properties of physics phenomena.

Spreadsheets can be used as specific-purpose software as well as for programming. Due to its structure and tools available in it, the amount of programming needed in a spreadsheet is minimal. A spreadsheet provides instant data storage of any type of data in the form of an extendable two-dimensional array of cells. This data can be used by a simple mechanism of referencing in terms of rows and columns. It is possible to apply algebraic and mathematical operations to the elements of the spreadsheet and these operations can be repeated, either interactively or by creating macros [6]. It is often done by formula editing and copying. This approach helps students to concentrate on analysis and interpretation of results rather than on time-consuming code debugging [7]. In Excel user can develop user defined functions using VBA and can be used these functions in cell structure of Excel and get their desired output directly [8].

In physics, students and teachers have to solve linear and non-linear differential equations to understand the laws of nature [9]. A spreadsheet program can be used to solve linear and non-linear differential equations in physics numerically and to obtain their visual graphical representations [10-13]. It may be also used for numerical integration techniques like Trapezoidal rule, Simpsons rule etc. When one solves an equation and analyzes the results, step by step, recording the successive values in the worksheet and plotting the results, then repeating the calculations with different input parameter values and

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comparing and analyzing the results we could take full advantage of various spreadsheet features [14]. Using spreadsheets animations and simulations in physics can be developed [15]. The spreadsheets can be used to visualize potential surfaces of charges as well as surface plots [16].

This paper presented spreadsheet implementation for obtaining the energies in perturbation of quantum harmonic oscillator and plotting of eigen functions with first and second order perturbation. Analytical solutions are used to plot the eigen functions in unperturbed state. Due to its abstract nature perturbation theory is difficult for students to understand. It is not possible for students to understand the perturbed eigen functions using only mathematical relations. The visual representations of unperturbed and perturbed eigen functions are necessary to make the concept clear. Scrollbars and naming facility to the cells are used to make the spreadsheet interactive.

Stationary State Perturbation Theory: Perturbation theory works best when the system's total energy is "perturbed" by a small additional potential energy. Consider the perturbation H' to the unperturbed Hamiltonian H_0 ***i.e.***

$$H = H_0 + \lambda H' \tag{1}$$

The eigen value equation satisfy the following equation [17]

$$H\psi_n = E_n \Psi_n \tag{2}$$

We will express the desired quantities as power series of λ as

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \lambda^3 E_n^{(3)} + ...$$
$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \lambda^3 \psi_n^{(3)} + ...$$

The eigen states and eigen energies of unperturbed state are assumed to be known. The eigen value equation is given by

$$H_0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

First order correction in energy is

$$E_n^{(1)} = \langle n^{(0)} | H' | n^{(0)} \rangle$$
$$E_n^{(1)} = H'_{nn} \tag{3}$$

which is the expectation value of H' evaluated in the nth unperturbed state.

The first order correction in eigen function is

$$\psi_n^{(1)}(\xi) = \sum_{m \neq n} C_{mn} \psi_m^{(0)} \tag{4}$$

where $C_{mn} = \dfrac{\langle m^{(0)} | H' | n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}} = \dfrac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}}$

The second order correction in energy is

$$E_n^{(2)} = \sum_{m \neq n} \frac{H'_{mn} H'_{nm}}{E_n^{(0)} - E_m^{(0)}} \tag{5}$$

If H' is Hermition, then

$$E_n^{(2)} = \sum_{m \neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}} \tag{6}$$

The second order correction in eigen function is

$$\psi_n^{(2)} = \sum_{i \neq n} d_{ni} \psi_i^{(0)} \tag{7}$$

where

$$d_{ni} = \frac{1}{E_n^{(0)} - E_i^{(0)}} \sum_{m \neq n} \frac{H'_{im} H'_{nm}}{E_n^{(0)} - E_m^{(0)}} - \frac{H'_{in} H'_{nn}}{(E_n^{(0)} - E_i^{(0)})^2} \tag{8}$$

Perturbation of Harmonic Oscillator: The potential energy for harmonic oscillator is

$$V = \frac{1}{2} kx^2$$

The Hamiltonian is given as

$$H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2$$

The perturbation is of the form

$$H' = \lambda x^k$$

where k = 1,2,3,4.

The Schrodinger's steady state equation for harmonic oscillator is given as

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left(E - \frac{1}{2}kx^2\right)\psi = 0 \tag{9}$$

The energy eigen values of harmonic oscillator are

$$E_n^{(0)} = \left(n + \frac{1}{2}\right)\hbar\omega$$

The unperturbed eigen functions are

$$\psi_n^{(0)}(x) = \left(\frac{\alpha}{2^n n!\sqrt{\pi}}\right)^{1/2} H_n(\alpha x) e^{-\alpha^2 x^2/2}$$

where n =0, 1,2,3,……

The classical limit is given as

$$x_0 = \sqrt{\frac{2E_n^{(0)}}{m\omega^2}} \quad (10)$$

It is convenient to simplify Eq. (9) by introducing the dimensionless quantities. Let us introduce dimensionless variable $\xi = ax$, we get

$$\frac{d^2\psi}{d\xi^2} + \left(2\varepsilon - \xi^2\right)\psi = 0 \quad (11)$$

Where $\alpha = \left(\frac{m\omega}{\hbar}\right)^{1/2}$ and $\varepsilon = \frac{E}{\hbar\omega}$.

The eigen functions are

$$\psi_n^{(0)}(\xi) = \left(\frac{1}{2^n n!\sqrt{\pi}}\right)^{1/2} H_n(\xi) e^{-\xi^2/2} \quad (12)$$

where $Hn(\hat{\imath})$ are Hermite polynomials of order n.

The classical limit in terms of dimensionless variable is

$$\xi_0 = \sqrt{2n+1} \quad (13)$$

The energy parameter is defined as

$$\varepsilon_n^{(0)} = \frac{E_n^{(0)}}{\hbar\omega}$$

Therefore,

$$\varepsilon_n^{(0)} = \left(n + \frac{1}{2}\right) \quad (14)$$

The perturbation in terms of dimensionless variable is

$$H' = b\xi^k$$

The first order correction in energy parameter is

$$\varepsilon_n^{(1)} = b\left\langle n^{(0)}\middle|\xi^k\middle|n^{(0)}\right\rangle$$
$$\varepsilon_n^{(1)} = b\xi_{nn}^k \quad (15)$$

The first order correction to the eigen function is

$$\psi_n^{(1)}(\xi) = b\sum_{m\neq n} C_{mn}\psi_m^{(0)} \quad (16)$$

Where $C_{mn} = \frac{\langle m^{(0)} | \xi^k | n^{(0)}\rangle}{\varepsilon_n^{(0)} - \varepsilon_m^{(0)}} = \frac{\xi_{mn}^k}{\varepsilon_n^{(0)} - \varepsilon_m^{(0)}}$

The second order correction in energy parameter is

$$\varepsilon_n^{(2)} = b^2 \sum_{m\neq n} \frac{|\langle m^{(0)} | \xi^k | n^{(0)}\rangle|^2}{\varepsilon_n^{(0)} - \varepsilon_m^{(0)}} \quad (17)$$

$$\varepsilon_n^{(2)} = b^2 \sum_{m\neq n} \frac{|\xi_{mn}^k|^2}{\varepsilon_n^{(0)} - \varepsilon_m^{(0)}}$$

The second order correction in eigen function is obtained by using equations (7) and (8).

The corrections in energies are $E_n^{(1)} = \frac{\varepsilon_n^{(1)}}{\alpha^k}$ and $E_n^{(2)} = \frac{\varepsilon_n^{(2)}}{\alpha^{2k}\hbar\omega}$

The energy is given as

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$$

Organization of Spreadsheet: The spreadsheet is prepared using MS Excel® 2007. In Excel it is easy to access to controls such as scrollbars because their implementation requires little or no macro programming [18]. The facility of naming a cell or range is available in Excel. Naming a cell allows us to reference it with that name instead of the default name. Naming the cell makes the formula easier because we don't need to remember exactly where the cell is in a workbook and we don't need to get into the whole nesting thing.

To obtain eigen function Hermite polynomials are required. These polynomials are obtained by user defined function HER(n,x) using VBA code [15].

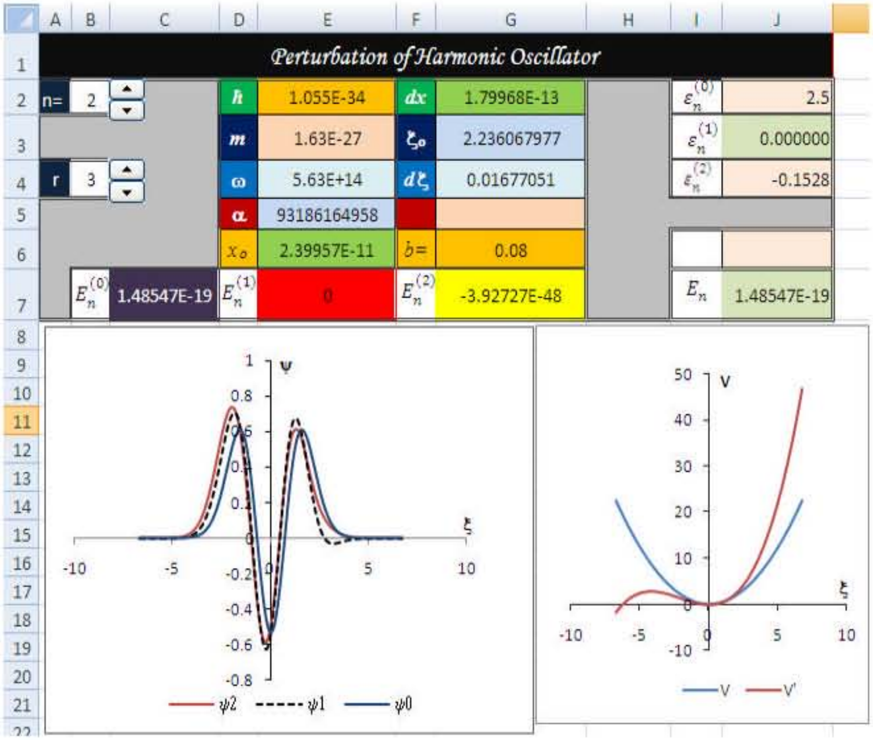

Fig. 1: Screenshot of sheet 1

The naming facility available in the excel is used to name the cells.

In Sheet 1 the cells named as:

B3: Named as n which takes value of order of the state. This is changed by scrollbar.

B4: Named as k which takes value index used in perturbation.

C7: Contains value of $E_n^{(0)}$ obtained by using formula = (n+1/2)*h*w in it.

E2: Named as h which takes value of Planck's constant h

E3: Named as m which takes value of mass

E4: Named as w which takes value of ù

E5: Named as alp which takes value of parameter α obtained by formula =SQRT(m*w/h) in it.

E6: Named as xo which takes value of classical limit obtained by equation (10).

G6: Named as b and contains the value of perturbation parameter.

The dataset in the spreadsheet on Sheet 2 is organized in the following way:

F1: The cell contains value of $d\xi$

A4: A404 is a column that contains the values for x by increment of dx from $-3x_0$ to $+3x_0$.

B4: B404 is a column that contains the values for ξ by increment of $d\xi$ from $-3\xi_0$ to $+3\xi_0$.

C4: C404 is a column that contains value of $\iota_n(\xi)$ which is obtained by using formula =SQRT(1/(FACT(n)*2^n*SQRT(PI())))*HER(n,B4)*EXP(-B4*B4/2) in cell C4 and pasting up to C404

F4: M404 contain eigen functions $\iota_0, \iota_1, \ldots\ldots \iota_7$ obtained by the same procedure as above for m = 0,1,…,8.

H413: O420: 8 × 8 matrix of $\langle m|\xi^r|n\rangle$ is formed in the following way:

In cell H413 to obtain ξ^r_{00} the formula used is =SUMPRODUCT(($B$4:$B$404)^k,($F$4:$F$404),(F$4:F$404)*$F$1)

In cell I413 to obtain ξ^r_{01} the formula used is =SUMPRODUCT(($B$4:$B$404)^k,($F$4:$F$404),(G$4:G$404)*$F$1)

By similar method all other matrix elements are obtained.

W413:AD420: The 8 × 8 matrix of $\varepsilon_n^{(0)} - \varepsilon_m^{(0)}$ is formed in these cells.

The coefficient C_{0n} is obtained in cell H426 by using INDEX and MATCH function over the arrays H413:O420 and W413:AD420.

	F	G	H	I	J	K	L	M	N	O
411						n				
412			0	1	2	3	4	5	6	7
413		0	0.75	0	2.1213203	0	1.224745	0	0	0
414		1	0	3.75	0	6.123724	0	2.738613	0	0
415		2	2.1213203	0	9.75	0	12.12436	0	4.743416	0
416		3	0	6.123724	0	18.75	0	20.12461	0	7.245688
417	m	4	1.2247449	0	12.124356	0	30.75	0	30.12474	0
418		5	0	2.738613	0	20.12461	0	45.75	0	42.124815
419		6	0	0	4.7434165	0	30.12474	0	63.75	0
420		7	0	0	0	7.245688	0	42.12482	0	84.75

Fig. 2: Screenshot of Matrix ξ^4_{mn} on Sheet 2. The values are rounded up to six decimal points.

For example to select ξ^r_{01} from the matrix the formula used is

=INDEX(H413:H420,MATCH(n,G413:G420,0))

To select $\varepsilon_0^{(0)} - \varepsilon_1^{(0)}$ from the matrix the formula used is

= INDEX(W413:W420,MATCH(n,G413:G420,0))

From I426 to O426 other coefficients C_{1n}, C_{2n}, C_{3n}, C_{4n}, C_{5n}, C_{6n} and C_{7n} are obtained by above procedure. Care has been taken that $C_{nn} = 0$.

The values of $\varepsilon_n^{(1)}$ obtained in the cell J428 and $\varepsilon_n^{(2)}$ in the cellJ430 respectively by selecting matrix elements from ranges H413:O420 and W413:AD420.

To obtain coefficient d_{nj} the equation (8) is used. For that purpose the integrals and energy differences are collected by INDEX and MATCH functions from arrays H413:O420 and W413:AD420.

The cells N434 to T434 contain coefficients d_{0n}, d_{1n}, ……. d_{7n}.

N4: N404 column contains the first order corrected in eigen function by using formula =C4+b*($H$427*F4+$I$427*G4+$J$427*H4+$K$427*I4+$L$427*J4+$M$427*K4+$N$427*L4+$O$427*M4) in cell N4 and pasting up to N404.

O4:O404 column contains the second order corrected eigen function.

RESULTS AND DISCUSSION

A spreadsheet program that has been developed for perturbation of harmonic oscillator is menu driven, user friendly and interactive. It allows the user to carry out a series of numerical experiments using different sets of parameters and to view the effect automatically in numerical and graphical form.

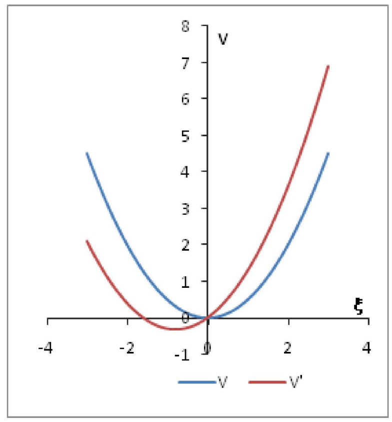

Fig. 3: Potential energy curves for b=0.8. Blue line shows unperturbed potential and red line shows potential with perturbation $b\xi$.

In this spreadsheet perturbation up to third excited state of harmonic oscillator are considered. If we want more states, we can obtain more eigen functions and increase order of matrix $\langle m|\xi^r|n\rangle$.

Consider the perturbation of the type $H' = bx$. The potential energy of the oscillator becomes $V' = \frac{1}{2}kx^2 + bx$ the potential parameter is $V' = \frac{1}{2}\xi^2 + b\xi$. The potential parabola is congruent to original parabola of $\frac{1}{2}\xi^2$. The new equilibrium occurs at $\xi = -b$ where the perturbation force is balanced by restoring force. This new potential minimum is lower than the original by the amount $-b^2/2$ [17].

All energy levels are equally depressed by the constant parameter $-b^2/2$. The centre of symmetry of new eigen functions is at at $\xi = -b$. The eigen functions are shown in the following Figure 4.

The energy parameter for different perturbations are listed in Table 1.

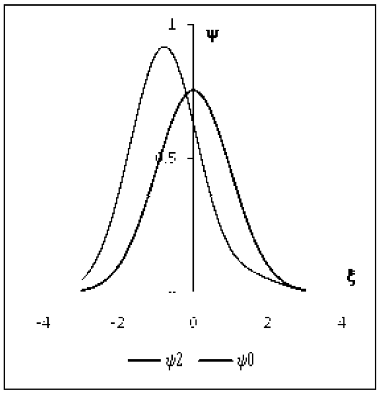

Fig. 4: The perturbed eigen function for $b\xi$ perturbation with $n = 0$, $b = 0.8$.

Table 1: Energy parameters for different perturbations

n	r	b	$\varepsilon_n^{(0)}$	$\varepsilon_n^{(1)}$	$\varepsilon_n^{(2)}$
0	1	0.8	0.5	0	-0.3197
0	2	0.05	0.5	0.02498945	-0.00062032
1	2	0.05	1.5	0.075	-0.001875
1	4	0.05	1.5	0.1875	-0.05156249
2	1	0.5	2.5	0	-0.12500008
3	3	0.05	3.5	0	-0.11593748
2	4	0.05	2.5	0.4875	-0.19218751

The first order perturbation is positive and energy is shifted up words. The second order perturbations are negative the energy levels are depressed when the n[th] level is below the other levels.

If an important level "m"-important in the sense of lying nearby, or of $\langle m|\xi^r|n\rangle$ being large-lies above the given level "n", then the second order shift is downwards; if it lies below, the shift is upward. We speak of this as a tendency of levels to repel each other [19].

The eigen functions for the harmonic oscillator can be plotted along with their first and or second order corrections for any b. Some examples of possible output are given in Figure 5 and 6 along with the parameters used to generate them.

In this spreadsheet perturbation up to third excited state of harmonic oscillator are obtained. If we want more states, we can obtain more eigen functions and increase order of matrix $\langle m|\xi^r|n\rangle$.

As part of learning process, it is useful to actually display the eigen functions with the dependence on applied perturbation and perturbation parameter. Understanding of the perturbation of harmonic oscillator can be deepened by posing questions such as

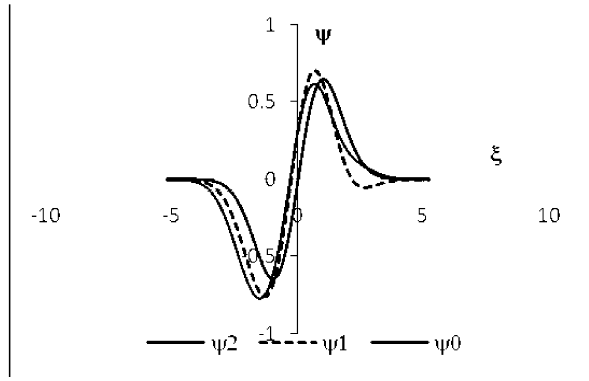

Fig. 5: The eigen function for n =1 state with perturbation $b\xi^3$ and b = 0.15. the blue-unperturbed, black dotted first order and red-second order.

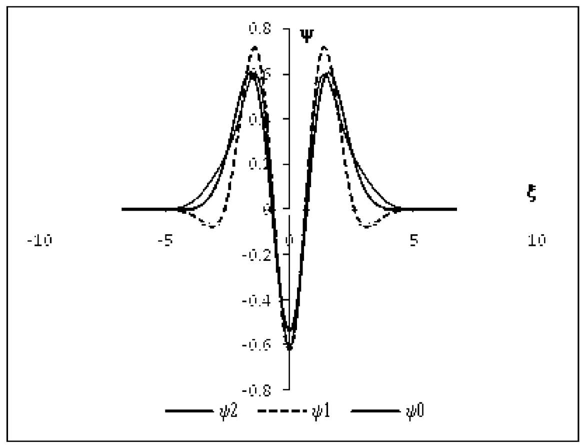

Fig. 6: The eigen function for n=3 state with perturbation $b\xi^4$ and b=0.06

"What would happen if we change perturbation keeping other parameters same?" or "What would happen to the eigen function and energy when state of the particle is changed?" By using such "what-if" questions, student can test their understanding of concepts and ideas of physical processes. This can all actually be tried with the spreadsheet animation. The use of spreadsheet in this way is supported by constructivist model of learning [20]. Before using spreadsheets, the students should be forced to tackle with the problem and writing down detailed predictions through thinking and discussion among themselves. The use of simulation then either confirms the correct thinking or forces a re-investigation to revise misconceptions.

CONCLUSIONS

The use of spreadsheets in perturbation of harmonic oscillator has been investigated. Details of using the spreadsheets in evaluating analytical solutions as well as providing the numerical solution of stationary state perturbation problems are outlined. Parameters can easily be changed and their effects investigated. The graphical abilities of the spreadsheets have been used in representing the obtained eigen functions and potential energy curves. The capability of Excel to define user defined functions using VBA is used for obtaining Hermite polynomials. The examples used here demonstrate that spreadsheet programs have proven to be an important pedagogical tool for a variety of problems in quantum physics education. These programs are very flexible, familiar and relatively easy to use. Spreadsheets can be used to model physical situations involving motion of particle and thus provide graphical representations to equations. With a variety of built-in mathematical functions and excellent graphics capabilities, the spreadsheet becomes a powerful instrument for modeling problems in quantum physics as well as in many areas of the physics. The problems that are modeled using spreadsheets are useful for teaching and learning. Spreadsheet simulations are effective for students learning because they provide both visual and kinesthetic experiences. They enhance students' ability of using mathematical experiences to study several phenomena of study and have a better understanding of how the input variables impact the dynamics of a problem. These simulations are also beneficial for those students whose logical and mathematical thinking is weak [20]. Students can easily learn to use spreadsheets in physics and this is good career training outside physics also. When students do physics with a spreadsheet, they benefit in two ways: (i) they enhance their learning ability by drawing connections between the language of mathematics and context of applications in physics; and (ii) gain a dynamic perspective and analytical power of this software tool to solve problems, develop understanding and explore concepts [12, 21, 22]. Also updating the contents of educational materials is easier in computer based instructions than traditional instructions [23].

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