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ARTICLE

Numerical Calculations of Energies for an Infinite Potential Well with Sinusoidal Bottom

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Abstract: We present an investigation for a particle confined in an infinite well with sinusoidal bottom, using the perturbation theory and numerical solution for the Schrödinger equation to obtain the eigen energies and wavefunctions. Potential strength and potential oscillation dependence of the state are examined and analyzed. It is shown that the particle in a box with sinusoidal bottom does not show up the Klauder phenomenon when the perturbations are gradually reduced to zero. The research results show that the potential oscillation significantly affects certain quantum states and, therefore, the ability to manipulate the energy difference between the states. In addition, our results for the present system converge to their corresponding values for the unperturbed one in the high-potential oscillation limit.

Keywords: Infinite well, Perturbation theory, Sinusoidal potential, Numerical calculations, Klauder phenomenon.

Introduction

Since the proposal of the infinite potential well as a hypothetical model set up to demonstrate the differences between both classical and quantum points of view regarding the movement of a free particle in some confinement, the research in this area never stopped. The infinite potential well was extensively studied under different constraints and modifications [1-5]. Even though the infinite potential well is a hypothetical model, it remains a good candidate for a lot of quantum applications [6-7], and its analytical solution is still widely used for variational and numerical techniques in quantum mechanics [8-9].

The traditional version of the infinite potential well (flat bottom) exhibits the well-known energy eigenvalues and normalized eigenfunctions given by:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2ML^2}, \Phi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right) \quad (1)$$

where M, L, and n denote the confined particle's mass, the well's width and the quantum number (n = 1, 2, 3, …), respectively. Changing the shape of the bottom of the well is expected to result in some modifications of the system's eigenvalues and the corresponding wave functions.

The sinusoidal potential is considered the general case for any periodic potential, since one can use Fourier series to write any periodic potential in terms of sine and cosine. Very recently, a prototypical model of a one-dimensional metallic monatomic solid containing non-interacting electrons was studied, where the potential energy has been considered to be sinusoidal [10]. Also, Sakly et al. [11] have investigated the electronic states using the

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sinusoidal potential for $Cd_{1-x}Zn_xS$ quantum dot superlattices with a finite barrier at the boundary.

In 2008, Alhaidari and Bahlouli [12] studied the infinite potential well with sinusoidal bottom and proposed an ability to get the exact energy eigenvalues from the solution of a three-term recursion relation. In their work, they also showed a possibility of the Klauder phenomenon (where the system for a certain perturbation will not give the same states as unperturbed Hamiltonian when the perturbation is turned off; mathematically:

$\lim_{\lambda\to 0}\langle H_0 + \lambda\, H'\rangle \neq \langle H_0\rangle$.

Three years later, Dhatt and Bhattachrayya [13] restudied the same system for the potential well by perturbative and variational methods and concluded the non-existence of Klauder phenomenon as perturbation goes to zero. Their work was carried out for the ground-state energy in the lowest perturbation orders by applying the standard Rayleigh-Schrödinger perturbation theory.

In the present work, the Schrödinger equation has been solved for the particle in an infinite well with sinusoidal bottom by using perturbative and numerical methods and the effect of the bottom potential parameters (potential oscillation and strength) on the energy and states of the particle has also been studied.

In the rest of this article, we present the theoretical framework and Hamiltonian in next section. Then, numerical calculations and illustrations are presented, and the last section is devoted for remarks and conclusions.

Theoretical Framework

The one-dimensional time-independent Schrödinger equation for a particle confined in an infinite square well with a cosine sinusoidal bottom is given by:

$$\left(-\frac{\hbar^2}{2\,m}\frac{d^2}{dx^2} + V(x)\right)\psi(x) = E\,\psi(x), \quad (2)$$

where

$$V(x) = \begin{Bmatrix} C\cos\left(\frac{k\pi x}{L}\right) & 0 < x < L \\ \infty & elsewhere \end{Bmatrix} \quad (3)$$

For the sake of simplicity, units are set such that $\hbar$ = 2m = 1.

Since the analytical solution of the above equation is not attainable and to obtain an approximate solution for this system, one can follow the perturbation-method steps. Dhatt et al provided a solution for the ground state with integer values of k [13] as:

$$E_1(k = 1, C) = \left(\frac{\pi}{L}\right)^2 - C^2\frac{L^2}{12\pi^2} + O(C^4) \quad (4)$$

$$E_1(k = 2, C) = \left(\frac{\pi}{L}\right)^2 - \frac{C}{2} - C^2\frac{L^2}{32\pi^2} + C^3\frac{L^4}{512\pi^4} + O(C^4) \quad (5)$$

$$E_1(k \geq 3, C) = \left(\frac{\pi}{L}\right)^2 - C^2\frac{L^2}{2\pi^2(k^2-4)} + O(C^4) \quad (6)$$

with the approximate ground-state wave function given by:

$$\Psi_1(k = 1, C) = \Phi_1 - C\frac{L^2}{6\pi^2}\Phi_2 + C^2\frac{L^4}{96\pi^4}\Phi_3 + O(C^3) \quad (7)$$

$$\Psi_1(k = 2, C) = \Phi_1 - C\frac{L^2}{16\pi^2}\Phi_3 + C^2\frac{L^4}{256\pi^4}\left[\Phi_3 + \frac{1}{3}\Phi_5\right] + O(C^3) \quad (8)$$

where Φ_i refers to the normalized parent box states given by:

$$\Phi_i = \sqrt{\frac{2}{L}}\sin\left(\frac{i\,\pi\,x}{L}\right). \quad (9)$$

To make a general view, we proceeded via a perturbative route:

$$E_n(C) = E_n^{(0)} + \langle\Phi_n^{(0)}|V|\Phi_n^{(0)}\rangle + \sum_{m\neq n}\frac{\left|\langle\Phi_m^{(0)}|V|\Phi_n^{(0)}\rangle\right|^2}{E_n^{(0)} - E_m^{(0)}} + O(C^3) \quad (10)$$

and obtained a closed-form correction (up to second order) for any quantum state energy with integer values of k with the help of the following integral relation:

$$\int_0^L \frac{2}{L}\sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{k\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\,dx = \begin{Bmatrix} -\frac{1}{2}\ if\ k = m+n \\ \frac{1}{2}\ if\ k = |m-n| \\ 0\ otherwise \end{Bmatrix} \quad (11)$$

where n, k, and m are positive integers.

The energy for any state (n) for a given integer (k) and strength (c) is given by:

$$E_n(c,k) = \frac{\pi^2 n^2}{L^2} - \frac{1}{2}\, c\, \delta_{k-2n} - \frac{c^2 L^2}{4\pi^2(k^2+2kn)} + \frac{c^2 L^2\,(1-\delta_{k-2n})\Theta\,(|k-n|-\epsilon)}{4\pi^2(2kn-k^2)} \qquad (12)$$

where ϵ is a small positive number to avoid the undefined value for the step function, $\Theta(0)$. For the ground state (n=1), Eq. (12) has been tested with previously mentioned Eqs. (4 - 6).

To be able to investigate the effect of larger values of *C* – where the perturbative approximated solution is not accurate – and the non-integer values of *k*, the Numerov numerical method was performed, and the eigen energies were calculated.

The Numerov method is a specialized integration formula for numerically integrating differential equations of the form:

$$\psi''(x) = f(x)\psi(x). \qquad (13)$$

For the time-independent 1-D Schrödinger equation,

$$f(x) = -\frac{2m(E-V(x))}{\hbar^2}. \qquad (14)$$

Choosing a grid spacing $\Delta x = x_i - x_{i-1}$, the integration formula is given by:

$$\psi_{i+1} = \frac{\psi_{i-1}(12-\Delta x^2 f_{i-1}) - 2\psi_i(5\Delta x^2 f_i + 12)}{\Delta x^2 f_{i+1} - 12} + O(\Delta x^6) \qquad (15)$$

And by shooting a trial energy and iteration over the grid domain, one can find the numerical energy and wavefunction. Interested readers can refer to [14].

Results and Discussion

In this section, we present our results for an infinite well with sinusoidal bottom and prefer to use L=1 in the numerical calculations.

To give a good picture about the sinusoidal bottom, we plot in Fig. 1 the infinite box for different values of *k*; so it is shown that the number of full waves (oscillations) equals $\frac{k}{2}$, and the even (odd) number of k exhibits a symmetric (antisymmetric) behavior around the middle point of the well $(\frac{L}{2})$,

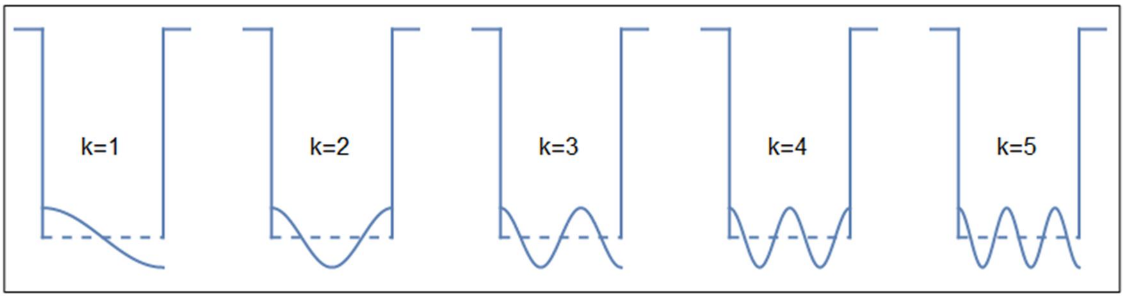

FIG. 1. Schematic plot of the infinite box for different integer values of *k*.

In Table 1, we provide the numerical value of energies for the ground state and few excited states for the particle in both cases, flat (unperturbed) and sinusoidal bottom well, for different values of potential amplitude (*C*) and potential oscillation (*k*), to show the agreement between the correlated energy (up to second-order correction) and quasi-exact numerical energy.

TABLE 1. Numerical values of energies (a.u) for the inner four states of the system, with L=1.

Quantum number	Energy		$E^{\text{perturbative}}$ $E^0 + E^1 + E^2$			$E^{\text{numerical}}$		
	Unperturbed energy		C= 2	C= 10	C=20	C= 2	C= 10	C=20
1	9.8696	K = 1	9.83583	9.02526	6.49223	9.83585	9.03972	6.70011
		K = 2	8.85694	4.55298	-1.39691	8.8571	4.57252	-1.24561
2	39.4784	K = 1	39.4919	39.8162	40.8294	39.4919	39.8015	40.6187
		K = 2	39.4699	39.2673	38.6341	39.4701	39.2676	38.6378
3	88.8264	K = 1	88.8322	88.9712	89.4054	88.8322	88.9714	89.4076
		K = 2	88.8328	88.9848	89.4597	88.8326	88.9652	89.3083
4	157.914	K = 1	157.917	157.994	158.235	157.917	157.994	158.236
		K = 2	157.917	157.998	158.251	157.917	157.998	158.248

Results show good agreement between the two methods, especially for low values of C, so the higher perturbative corrections can be neglected. Meanwhile, for larger values of C (when the perturbation becomes comparable to the ground-state energy), the effect of higher-order corrections becomes significant for ground state (n = 1) and less significant for higher states (n > 1), which agrees with the limitation of perturbation method. For a given value of C, the higher states are less sensitive to perturbation than the lower states. From this point of view, one can conclude that the perturbation method is suitable to investigate this problem for small values of C and so numerical calculations lead to a more reliable result for this reason, the Numerov numerical method has been used to produce all the following illustrations, while the perturbation analytical expressions for energy have been considered for some explanations.

The ground-state energy has been plotted in Fig. 2 as a function of the bottom potential amplitude for different integer values of k (the k = 2 case has been plotted separately in Fig. 2b). Fig. 2a clearly shows that as k increases, the effect of the perturbation becomes less significant and the ground-state energy becomes closer to the unperturbed one; notice k = 60 case. Eq. (12) shows that the first-order correction equals zero for any integer value of k, except for (k = 2); so, it is expected that all major corrections come from the second-order correction term. As it is known, the second-order correction of the ground state always reduces the energy of the ground state. In contrast to the above remarks, the ground-state energy for (k = 3) is less than (k = 1) energy.

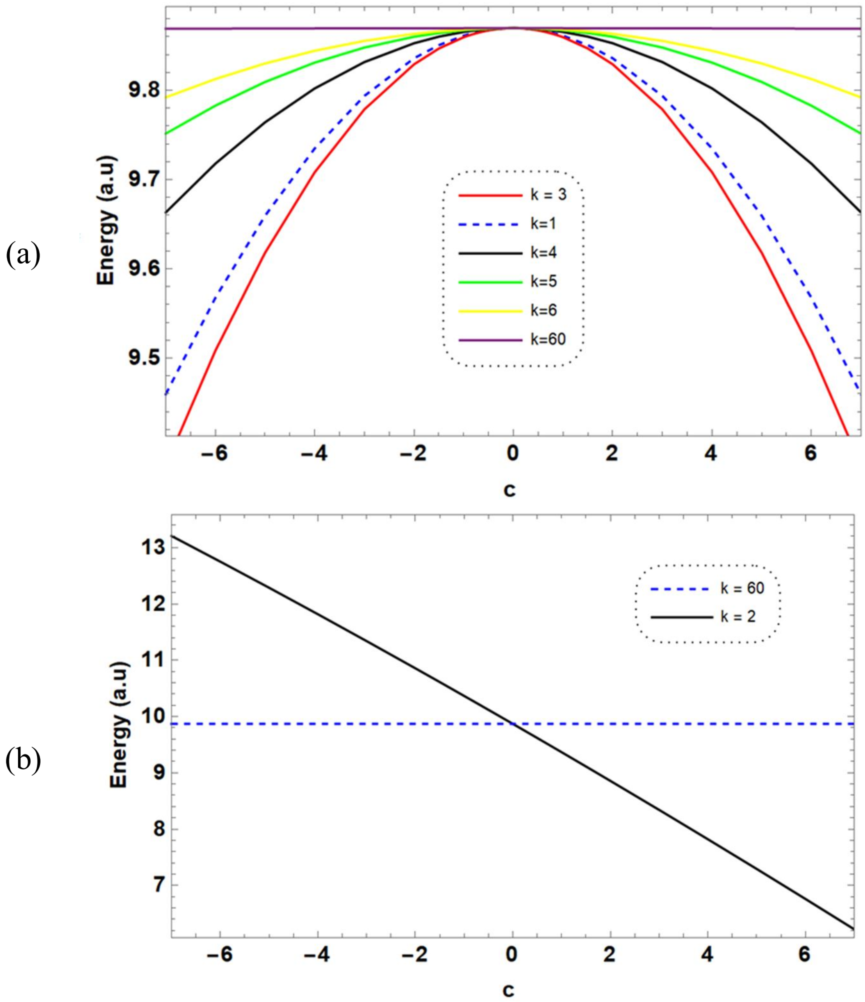

FIG. 2. Ground-state energy *versus* the perturbation strength c, for different values of k.

For Fig. 2b, the k = 2 case, the major contribution comes from the first-order correction; so, the curve shows a linear dependence between the ground-state energy and C with a slope almost - $\frac{1}{2}$.

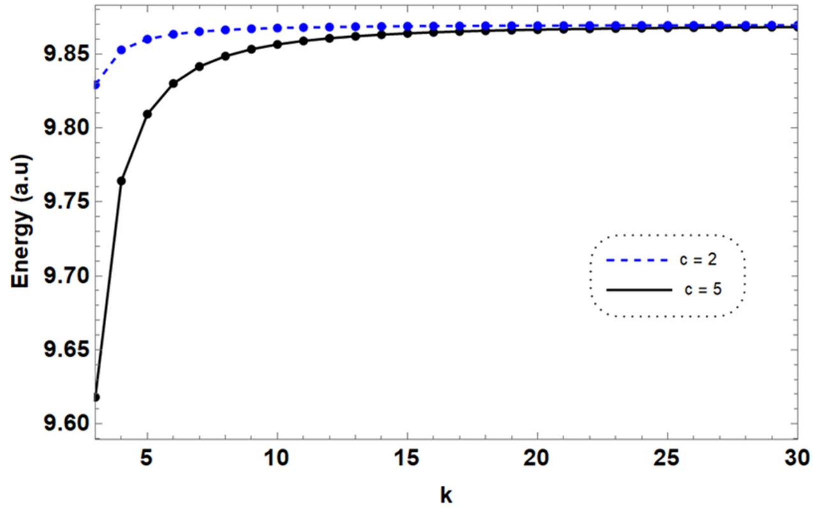

FIG. 3. Ground-state energy as a function of *k* for different values of *C*.

To ensure the above discussion for large values of *k*, the ground-state energy as a function of *k* for two values of *C* has been plotted, as shown in Fig. 4. The plot shows the independence of energy on the value of *C* as *k* increases. This is due to the very large number of oscillations (or wavelengths) in the well, which means that there is no enough time for the electron to catch up with the perturbation, leading to the flat bottom potential solution.

Now, for the higher state, for example, n = 2 (see Fig. 4).

(a)

(b)

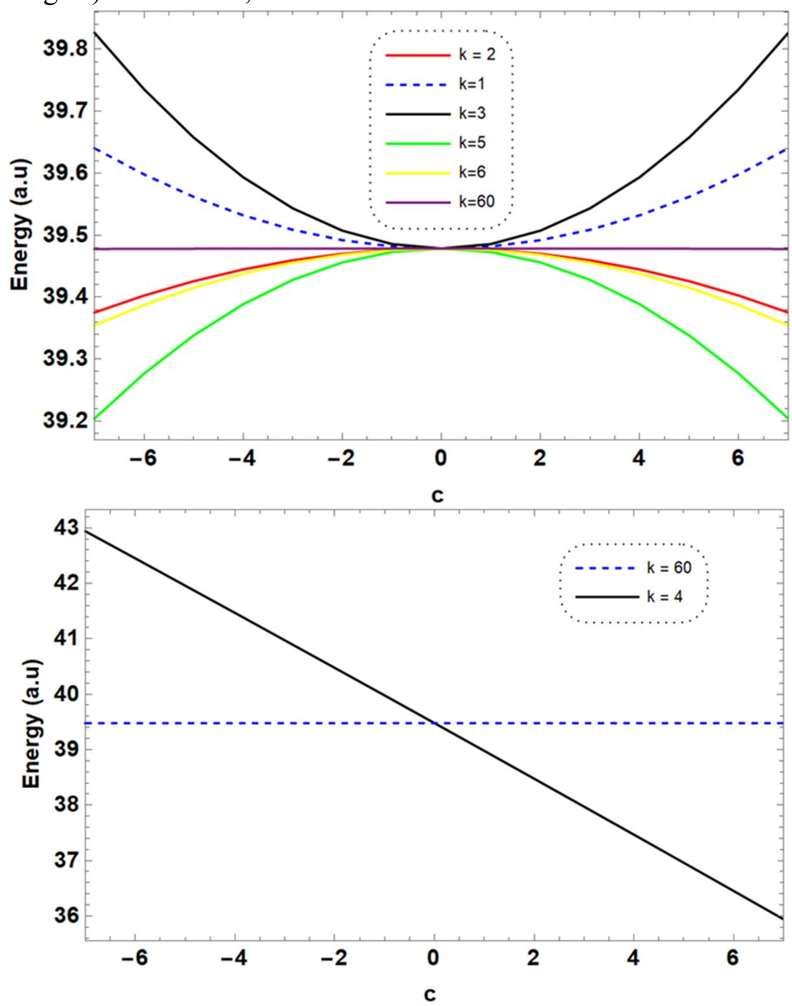

FIG. 4. Energy as a function of *C* for different values of *k* for the first excited state.

For the sake of comparison with previously published work [12], we plot the total state in the same unit as ref. [12], where the plot exactly matches the previous one for k=1, which shows no Klauder phenomenon. From Fig. 4, in that reference, there are extra nodes in n = 1 and n = 2. To ensure this here, we plotted the wave function for the two cases $k = 1$ and $k = 2$; no any further node has appeared.

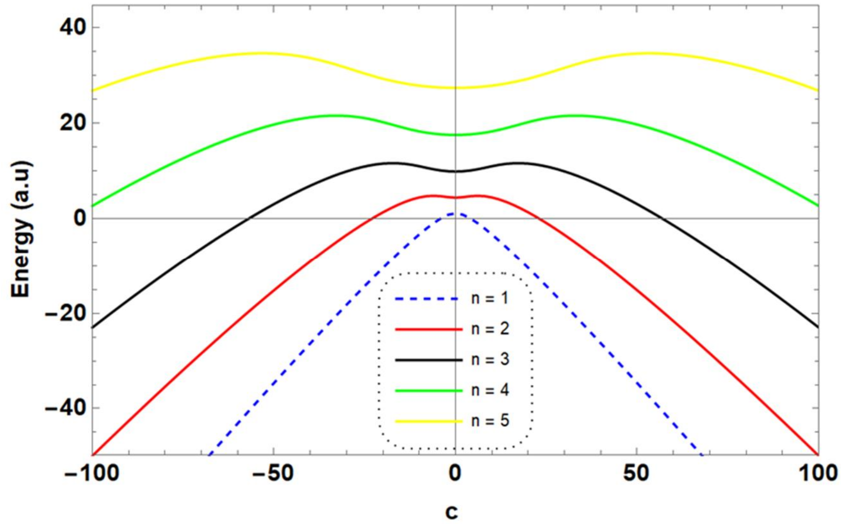

FIG. 5. Energy spectra as a function of C, for $k = 1$.

(a)

(b)

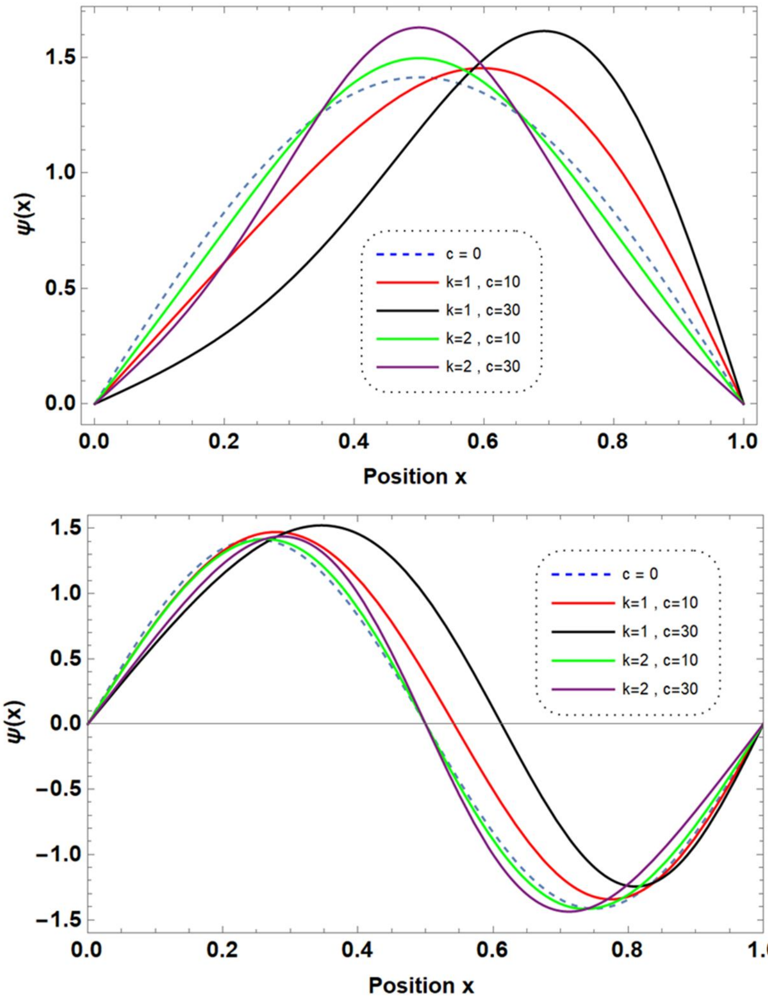

FIG. 6. Normalized wave function for the ground state (a) and first excited state (b), for different values of k and C.

As a final illustration, we study the case for non-integer k and give 3 plots. Again, the plots show that the system does not feel the perturbation after a certain value of *k*, which means that when the number of oscillations becomes large enough, the system has no enough time to adjust itself due to perturbation.

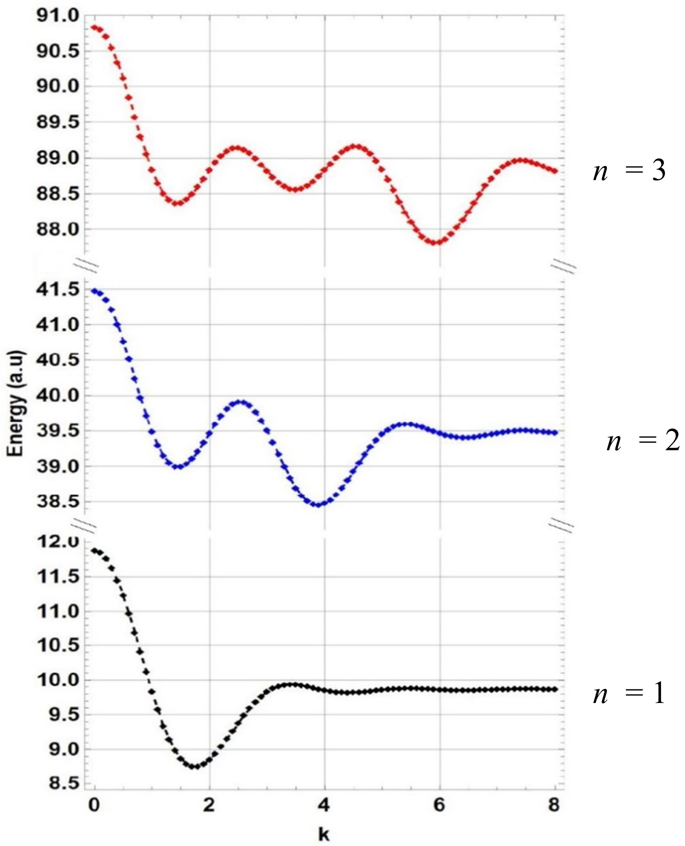

FIG. 7. The lowest eigen energies as a function of *k*; here *k* is taken from 0 up to 8, with steps of 0.1.

Conclusions

In this work, we calculated the energies and wavefunctions for the infinite well with sinusoidal bottom using numerical and perturbative methods. The effect of the potential oscillation and amplitude of the perturbation on the energies of the ground and excited states was examined. For each of the two selected frequencies (k = 1 and 2), it was found that the ground-state energy decreases as the amplitude of the perturbation increases, but the energy of an excited state increases as the amplitude increases, with the exception for the first excited state when $k = 2$. Our results also showed that as the oscillation of the perturbation increases, the energies of all states get closer to their corresponding values for the unperturbed well, and for very high frequencies, the energies converge to their corresponding values for the unperturbed well. In this case, the perturbed system does not have the time to catch up with the perturbation; thus, the system behaves as if the bottom of the well is flat. In addition, an important conclusion of our results is that the sinusoidal bottom well does show the Klauder phenomenon. An additive value of this work is the ability of exact calculations of the energy eigenvalues for the infinite well with sinusoidal bottom using numerical methods. This work is a constructive illustration for the application and usefulness of exact numerical and perturbation methods in studying simple but illuminating systems.

It may also be interesting to know how the ground-state energy depends on the perturbation for large *k*. Actually, the large-*k* limit is particularly significant because we expect on physical ground that too many oscillations of a cosine function over a finite domain should average out to zero [15]

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