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The effects of the variable mass on the electronic and nonlinear optical properties of octic anharmonic oscillators

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Abstract In this paper, we investigate theoretically the effects of a spatially varying effective mass distribution on the electronic and optical properties of octic anharmonic oscillators. Calculations to determine eigenvalues and eigenfunctions of the electron are performed within the effective mass approximation by using the diagonalization method. Optical absorption coefficients are obtained from the two-level approach in the density matrix expansion. Numerical results show that the position-dependent effective mass has a significant effect on the electronic energies and transitions between the subbands in single and double octic anharmonic oscillators. Furthermore, it was found that the optical properties of the system can be tailored in accordance with the desired purpose by changing the structural parameters of the system determining the size and the shape and with a proper choice of effective mass distribution.

1 Introduction

The quantum harmonic oscillator (HO) is a fundamental model in quantum mechanics that describes the behavior of a particle in a potential that is quadratic in its displacement from equilibrium. An anharmonic oscillator (AHO) potential is defined with the potential function that deviates from the harmonicity and these potentials have applications in various areas of physics, including molecular and solid-state physics. The eigenvalues and eigenstates of an AHO potential can be obtained using both analytical and numerical methods. Analytical methods involve solving the Schrödinger equation for the anharmonic potential by making approximations or using perturbation theory. Numerical methods involve using algorithms to solve the Schrodinger equation numerically.

Overall, AHO potentials are of great interest to scientific researches due to their important role in the evolution of many branches of quantum physics. Both numerical [1–9] and analytical techniques [10–13] have been used to study these potentials, and they have found applications in a wide range of fields, including molecular and solid-state physics. As is known, anharmonic oscillators are often encountered in molecular vibrations where the potential energy function is not entirely quadratic but contains higher-order terms that describe deviations from ideal harmonic behavior. Diatomic molecules are oscillatory systems in which nuclei vibrate around their equilibrium positions, and the vibrational motion of these systems is often modeled using the harmonic and anharmonic oscillator potentials, depending on the accuracy of the model. In this context, when studying the vibrational motion of diatomic molecules in quantum mechanics, the potential energy function describing the interaction between two atoms must include higher-order terms such as sextic, octic, and decatic. Non-harmonic effects become important at high vibration energy levels, where deviations from the harmonic approximation become more pronounced. Furthermore, AHO potentials with higher-order anharmonic terms have been extensively studied because they play an essential role in quantum tunneling time problems and molecular spectra [14–22]. The restrictions on the movement of particles confined within the low-dimensional semiconductor materials which have different size and shape very clearly affect the linear and nonlinear optical properties of materials such as absorption, refractive index changes, second- and third-harmonic generations of the semiconductor heterostructures, and these properties are of great importance in the productions and applications of optoelectronic devices such as high-speed electro-optical modulators, optical switching, infrared photo-detectors, semiconductor lasers, and far-infrared laser amplifiers [23–30]. By changing the structure parameters of low-dimensional semiconductor materials such as shape, size, width, and depth, as well as applying external fields such as electric, magnetic, and intense laser fields, the electronic, linear, and nonlinear optical properties of these materials can be appropriately tuned. Therefore, since the nonlinear optical effects of low-dimensional semiconductor materials are a hot topic for both theoretical and experimental research, the linear and nonlinear optical properties of these materials have been and will continue to be intensively studied [31–35].The octic AHO is a theoretical model used in quantum mechanics to study the behavior

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