Anharmonic Potential

O.L. Santos-Pereira

e-mail: osvaldo.pereira@sciencedata.ai

Abstract

Anharmonic Potential

1 Anharmonic Potential

Considering a particle in a Anharmonic Potential, where the Hamiltonian is given by $H = H_0 + W$, and the perturbation is a quartic potential given by $W = \lambda x^4$, where λ is a constant, and remembering that the unperturbed Hamiltonian for the harmonic oscillator is given by

$$H = \frac{P^2}{2m} + \frac{1}{2}kx^2. \tag{1.1}$$

The range of applications for this type of potential well ranges from biology, chemistry, and quantum field theory. When $k < 0$, then the potential has two minima. This problem is know as the double potential well. Applying the perturbation theory formulas, then the first order corrections to the n'th energy level is given by the following equation,

$$E_n^{(1)} = \frac{3\hbar^2}{4m^2\omega^2}\lambda(2n^2 + 2n + 1) \tag{1.2}$$

The harmonic oscillation is a good approximation for molecular vibration, but has some limitations. Due to equal spacing of energy level, all transitions occur at the same frequency, however experimentally many lines are often observed, called overtones. The harmonic oscillator does not predict bond dissociation, that means you cannot break it no matter how much energy is address. Anharmonic oscillation is defined as the deviation of a system from harmonic oscillation, is described as the restoring force is no longer proportional to the displacement.

References

[1] Cohen-Tannoudji, Quantum Mechanics, vol.2. Appendix of chapter XI, page 1.110 (page 229 on djvu file)

[2] David J. Griffiths, Quantum Mechanics. Chapter 6, page 249.

[3] Doron Cohen, Lectures on Quantum Mechanics. (page checked on 08/29/2018). His lecture notes in pdf file on arxiv. And the pool of problems are here. Check this one.

[4] George Siopsis, Quantum Mechanics course (page).