Modulation of Diatomic Molecular Spectra by Gravitational Waves

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Abstract

Gravitational waves (GWs), ripples in spacetime propagating at the speed of light, have reshaped our understanding of the cosmos since their first detection in 2015. These waves offer a unique observational probe of astrophysical phenomena otherwise inaccessible through traditional electromagnetic methods, such as binary black hole mergers. While currently detected GWs predominantly fall below 10 kHz, higher-frequency signals—potentially originating from exotic theoretical sources or early Universe processes—remain undetectable with existing instruments. In this work, we explore the interaction of GWs with diatomic molecular vibrations, illustrating in principle how such effects could imprint subtle signatures on molecular spectra. Using first-order perturbation theory, we calculate the energy level shifts induced by GW interactions in diatomic molecules modeled by the Morse oscillator potential. These shifts lead to small modifications in vibrational spectral lines, providing a theoretical basis for studying GW-induced perturbations in molecular systems.

Introduction

Gravitational Waves (GWs):
- First proposed in 1975 for atomic effects [1]; first detected in 2015 [2].
- Confirmed Einstein's general relativity as ripples in spacetime.
- GWs stretch and squeeze space as they propagate at the speed of light.

GW Sources & Detection:
- Generated by black holes, neutron stars, and white dwarfs.
- Different sources emit different frequencies (nanohertz to kilohertz).
- High-frequency GWs remain undetectable with current instruments.

Diatomic Molecules & GW Effects:
- Chosen as test particles due to their response to GWs.
- Stronger GW effects occur when objects are far apart.

Spectroscopy & Energy Shift Analysis:
- Uses Harmonic oscillator and Morse oscillator models.
- Studies the vibrational spectra of diatomic molecules under GW influence.
- Perturbation theory applied to calculate energy shifts.

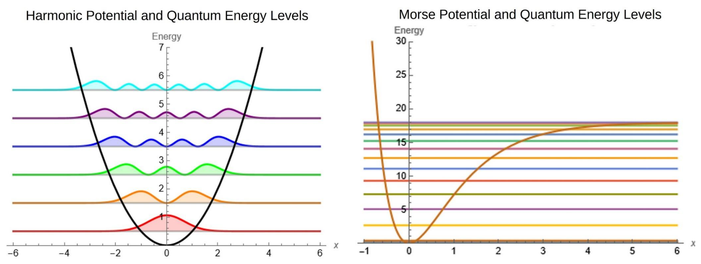

Fig.1 Difference Between Harmonic and Morse Potentials

Objectives

- To investigate the impact of gravitational wave interactions on the vibrational of diatomic molecules
- To explore the potential applications of these discoveries to practical astronomical observations

Calculation and analysis

Harmonic Oscillator

The Schrödinger equation of the harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x)+\frac{1}{2}m\omega^2x^2\psi(x)=E\psi(x)$$

Wave function of the harmonic oscillator:

$$\psi_n^{(0)}(x)=\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^n n!}}e^{-\frac{m\omega x^2}{2\hbar}}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

Eigenenergy:

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

First order eigenenergy:

$$E_n^{(1)}=\left\langle\psi_n^{(0)}\middle|H'\middle|\psi_n^{(0)}\right\rangle=\int_{-\infty}^{\infty}\left(\psi_n^{(0)}\right)^*H'\psi_n^{(0)}dx$$

The GWs Hamiltonian:

$$H'=\frac{1}{4}m\omega_{gw}^2Acos(\omega_{gw}t)(\ell_0+x)^2$$

First order corrections of energy for $n=0,1,2,3$:

$$E_0^{(1)}=\frac{A(\hbar+2\ell_0^2m\omega)\omega_{gw}^2\cos(\omega_{gw}t)}{8\omega}$$
$$E_1^{(1)}=\frac{A(3\hbar+2\ell_0^2m\omega)\omega_{gw}^2\cos(\omega_{gw}t)}{8\omega}$$
$$E_2^{(1)}=\frac{A(5\hbar+2\ell_0^2m\omega)\omega_{gw}^2\cos(\omega_{gw}t)}{8\omega}$$
$$E_3^{(1)}=\frac{A(7\hbar+2\ell_0^2m\omega)\omega_{gw}^2\cos(\omega_{gw}t)}{8\omega}$$

First order corrections of energy for any of n :

$$E_n^{(1)}=\frac{1}{4}\frac{A}{\omega}\omega_{gw}^2\cos(\omega_{gw}t)\left[\left(n+\frac{1}{2}\right)+\frac{\ell_0^2m\omega}{\hbar}\right]$$

Total energy of the harmonic oscillator:

$$E_n=\left(n+\frac{1}{2}\right)\hbar\omega+\frac{1}{4}\frac{A}{\omega}\omega_{gw}^2\cos(\omega_{gw}t)\left[\left(n+\frac{1}{2}\right)+\frac{\ell_0^2m\omega}{\hbar}\right]$$

Consider the spectrum of the harmonic oscillator that results from the energy transition from the excited state n to the ground state

$$f_{n\to0}=\frac{E_n-E_0}{\hbar}$$

for $n=1,2,3$:

$$f_{1\to0}=2\omega+\frac{A\omega_{gw}^2cos(\omega_{gw}t)}{4\omega}$$
$$f_{2\to0}=4\omega+\frac{A\omega_{gw}^2cos(\omega_{gw}t)}{2\omega}$$
$$f_{3\to0}=6\omega+\frac{A\omega_{gw}^2cos(\omega_{gw}t)}{4\omega}$$

The spectrum frequency for any of n

$$f_{n\to0}=\left(2+\frac{A\omega_{gw}^2cos(\omega_{gw}t)}{4\omega^2}\right)n\omega$$

The spectrum wavelength for any of n

$$\lambda_{n\to0}=\left(\frac{4\omega}{2+A\omega_{gw}^2cos(\omega_{gw}t)}\right)\frac{c}{n}$$

Discussion and Conclusion

For the harmonic potential when diatomic molecules are perturbed by GW affects energy and spectrum which are related to GW as follows

Energy shift and Total energy
- Directly proportional to the Bond length (ℓ_0), the reduced mass of the diatomic molecules (m) and the angular frequency of the GW (ω_{gw})

Spectrum
- The original spectral frequency changes and is directly related to the angular frequency of the GW (ω_{gw}).

Reference

[1] N. Wanwieng, N. Chattrapiban, and A. Watcharangkool, "The effects of gravitationalwaves on a hydrogen atom," Classical and Quantum Gravity, vol. 40, no. 23, p. 235004,2023.

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