Diatomic Molecular Vibration in a Strong Gravitational Field

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1 Introduction

Within diatomic molecules, the two atoms execute periodic vibrations around a fixed center of mass, having one rotationless ground mode of vibration due to stretching or compression along a single bond. In first approximation, such motion is simplest—exhibiting harmonic motion—where the vibrational energy is a quadratic function of the internuclear distance with respect to equilibrium [1]. Then, all overtones will have frequencies with integer multiples of the fundamental frequency produced by the diatomic molecules. However, in practise, molecular vibrations are only harmonic at the smallest scale, since the excitation states of the higher overtones have progressively lesser energies than the predicted multiples of the ground state, up to the point when the molecule will break apart. Consequently, at higher energies and for larger diatomic displacements, the underlying potential energy takes the form of the Morse potential [2, 3], accurately describing anharmonic nuclear vibrations and bond dissociations.

2 Methods

In the present work, we extend a recent study of the relativistic harmonic oscillator in a gravitational field [4] to a model which describes the vibrational spectra of rotationless diatomic molecules including relativistic effects—in particular the effects of strong uniform gravity. The mathematical formalism relies on the initial work of the relativistic brachistochrone [5], which later on was also applied to the case of the relativistic pendulum [6, 7].

Here, we use the Euler-Lagrange approach for relativistic dynamics [8] with a Morse/long-range potential energy function to derive the equations of motion characterizing the vibrational behaviour of the diatomic molecule within a uniform gravitational field. Significant difficulties arise in the analytical treatment of the corresponding relativistic gravitational potential, which is one of the key elements in the derivation. Thus, the final analysis of the diatomic vibrational modes becomes too complicated to evaluate in fully closed form.

3 Results and Conclusions

By utilizing numerical integration and providing a few representative estimates of the model, we can simulate the dynamics of the diatomic system illustrating some of its most important features.

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It is expected that these predictions could be relevant for the detection of strong gravitational fields in the context of radiation astronomy.

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