Diatomic Molecular Vibrations in Intense Laser Fields: An Analytical Perspective

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Diatomic molecules subjected to intense laser pulses exhibit a range of nonlinear interactions, strongly dependent on the relationship between laser parameters and molecular properties. While theoretical models for molecular interactions with laser fields are well established, analytical approaches in the strong-field regime remain scarce and often rely on approximations, whereas numerical methods become increas-ingly costly for infrared (IR) wavelengths [1,2].

In this contribution, we introduce a general mathematical framework to describe a Morse potential under intense IR excitation. Our approach incorporates both permanent and field-induced dipole moments, along with their gradients, into the Hamiltonian, validated through density-functional theory calculations. Consequently, our model is applicable to both homonuclear and heteronuclear diatomic molecules, as well as certain alkali metal dimers. As a demonstration, we apply our method to H_2 and LiH, showing that an IR laser field in the intensity range significantly shifts vibrational levels (see Fig. 1) and alters the equilibrium internuclear distance. Our results reveal that the dipole gradient and polarizability gradient play a crucial role in these effects. We derive exact analytical expressions for vibrational energy levels and bond-length modifications within the Kramers-Henneberger frame, valid across a broad wavelength range [3].
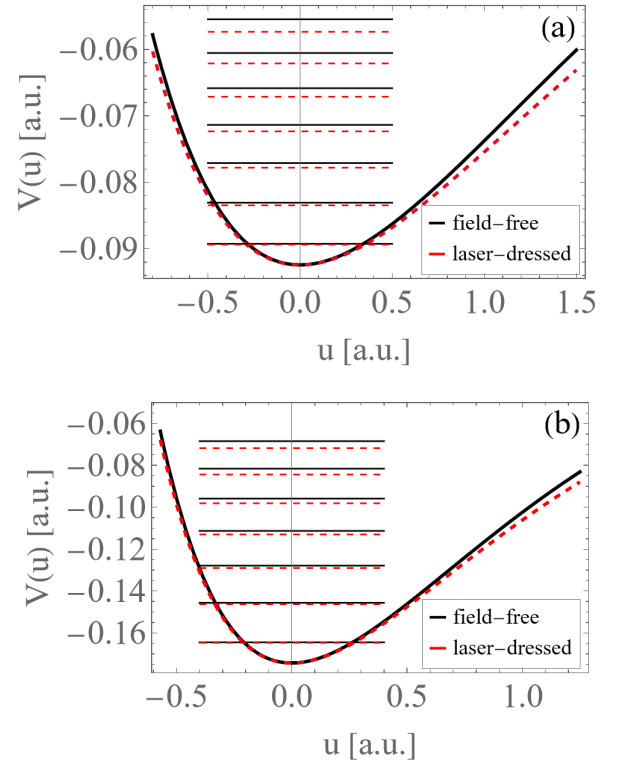

Figure 1: Field-free (black solid curve) and laser-dressed (red dashed curve) Morse potentials of LiH (a) and H_2 (b). The horizontal lines indicate the first seven energy levels for each potential, following the same line styles. The applied laser parameters are $I_0 = 2.8 \times 10^{13}$ W/cm^2 and $\lambda = 1500$ nm

References

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