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Lennard-Jones Oscillations in an Elastic Environment

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Abstract

In this purely analytical analysis, we have investigated the effects of a point-like defect in a continuous medium on a diatomic molecule under the influence of small oscillations arising from the Lennard-Jones potential. In the search for bound-state solutions, we have shown that the allowed values for the lowest energy state of the molecule are influenced by the presence of the defect. Furthermore, another quantum effect was observed: the stability radial point of the diatomic molecule depends on the system's quantum numbers; it is quantized.

Keywords: point-like defect; Lennard-Jones potential; small oscillations; solutions of the bound states

MSC: 81T45; 81T20; 81Q05; 81Q70

1. Introduction

The Lennard-Jones potential (LJP) is a key concept in physics and chemistry that describes how two neutral atoms or molecules interact. It models their potential energy as a function of distance, offering a straightforward approach to understanding non-bonding interactions. The model is governed by two forces: a strong repulsive force at short range that prevents atomic overlap, and a weaker attractive force at longer range. The LJP effectively illustrates the balance between these opposing forces. An important model in condensed matter physics and molecular dynamics, the LJP [1] is frequently employed as an explanation for interactions between neutral atoms or molecules. Particles controlled by the LJP display fascinating oscillatory behaviors when embedded in an elastic environment because of the interaction of repulsive and attractive forces. Together with the restoring forces imposed by the elastic medium, these oscillations result from the balance between the LJP's steep repulsion at short distances and its weaker attraction at intermediate ranges. The stiffness in the medium, damping effects, and exterior disturbances all affect the LJ oscillations in an elastic environment. Complex periodic or quasi-periodic motion can result from the elastic matrix's additional restoring forces, which can alter the particles' equilibrium positions and vibrational modes. According to studies, depending on the system parameters and initial conditions, these systems may display harmonic, anharmonic, or even chaotic oscillations. These phenomena have been investigated through theoretical and computational analyses, such as continuum approximations and molecular dynamics simulations. Potential models are proposed to describe molecules and their clusters, with the aim of characterizing them and obtaining their chemical and physical properties [2].

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One well-known potential model for describing diatomic molecules (homonuclear or heteronuclear) is the Mie-type potential energy model [3,4], from which the Kratzer–Fues [5,6] and LJ [7,8] potentials can be derived.

In particular, the LJP [6,7] is one of the most successful and applied models in various areas of physics, including atomic–molecular physics. The LJP roughly describes a molecule composed of two atoms, in which there is a repulsive force between the atoms at small separation distances, which prevents them from overlapping, and an attractive force at large separation distances, which ensures the chemical bonding of the atoms in the diatomic molecule. At some distance between the atoms that make up this diatomic molecule, these forces are in equilibrium.

LJP has been investigated in solids, for example, in porous materials [8] and disordered solids [9], as well as in liquids [10,11]. This potential has also been used to study the assembly of antiphyles with tethered nanoparticle formats [12], on thermal conduction in classical low-dimensional lattices [13], and in the modeling of noble gases [14]. It is worth noting that the latter, the noble gases, have wide applications in aerospace engineering. For example, helium is used in cooling systems for sensitive equipment in aircraft and satellites, while xenon and krypton are used as propellants in ion thrusters, which are electric propulsion systems used in spacecraft [15]. Argon, on the other hand, is used in inert atmospheres to protect aircraft and spacecraft components during welding and manufacturing processes [16].

Investigations in the field of atomic molecular physics involving the LJP are restricted to computational modeling or numerical calculation, as its mathematical structure does not make analytical treatment possible, both in the classical [17] and quantum contexts [18]. One possible way to approach this potential analytically is to treat it in a particular regime, that is, in a regime of small oscillations. As mentioned above, the LJP has a stability point, meaning that the repulsion and attraction forces, at a specific radial point between the atoms that make up the diatomic molecule, cancel each other out. Therefore, around this point, the LJP behaves like a harmonic oscillator. In this case, in analogy to the Schrödinger oscillator, it would be possible to analytically solve the LJP in the regime of small oscillations.

Small oscillations have been investigated in some quantum mechanical systems, for example, in a 2D ring [19], on a diatomic molecule under effects to the global monopole [20], on Kratzer–Fues potential in a medium with a point-like defect [21], and on Morse potential in an elastic background [22]. The potential of harmonic oscillator goes far beyond mere academic practice, as several physical properties arise from vibrations, for example, vibrations in molecules and atoms, magnetic properties in solids that involve vibrations in atomic nuclei, and thermal and acoustic properties that arise from atomic vibrations [23].

The structure of this paper is as follows: in Section 2, we present the Schrödinger equation rewritten in a nontrivial background characterized by the presence of a point-like defect; in Section 3, we analyze the LJP in the regime of small oscillations; in Section 4, we determine solutions of bound states for a quantum system defined by a diatomic molecule under effects of Lennard-Jones oscillations in the presence of point-like defect; in the Section 5, we present our conclusions.

2. Radial Schrödinger Equation in an Elastic Background

To effectively analyze a non-relativistic quantum system set against a rich background defined by geometric or topological complexities, it is essential to utilize the Schrödinger equation in the framework of the Laplace–Beltrami operator. This approach not only clarifies the system's behavior but also reveals the profound interplay between quantum mechanics and the underlying geometry of the space.

$$-\frac{\hbar^2}{2m}\nabla^2_{LB}\Psi(\vec{r},t)+V(\vec{r},t)\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}, \tag{1}$$

where $\hbar = h/2\pi$, with h being the Planck constant, m is the diatomic molecule mass, $V(\vec{r}, t)$ is the potential energy to which the molecule is submitted, and

$$\nabla^2_{LB} = \frac{1}{\sqrt{g}}\partial_i(\sqrt{g}g^{ij}\partial_j) \tag{2}$$

is the Laplace–Beltrami operator. It is worth noting that the metric matrix g provides information about the medium's geometry.

In this discussion, we examine an elastic environment characterized by a curved background resulting from the presence of a point-like defect (PD). This defect can manifest as either an impurity or a vacancy [24], significantly influencing the properties and behavior of the medium. The mechanism for producing this defect is known as the Volterra process [25] or "cut and paste" process, which, in short, is carried out in three parts [24]: (1) cut a sphere in half; (2) remove its interior; (3) then shrink the sphere until it forms a point. In this case, we have a point defect in the continuous elastic medium: a vacancy. An alternative approach to executing this mechanism involves adding matter rather than removing it. This process still results in a point defect, but it now presents itself as an impurity within the continuous elastic medium. This insight highlights the nuanced ways in which matter can interact within a system, emphasizing the significance of impurities in shaping the properties of the medium.

This type of geometric defect is analogous to the topological defect predicted in cosmology and gravitation known as a global monopole [26–28]. Therefore, this defect has been investigated in various branches of physics [29–33]. In particular, within quantum mechanics, there are studies in both relativistic and non-relativistic cases. In the first case, we have studies on scalar bosons [34], in exact solutions of the Klein–Gordon equation in the presence of a dyon magnetic flux and scalar potential [35], quantum oscillators [36], hydrogen and pionic atoms under effects of harmonic oscillations [37], and on a scalar particle in a wormhole [38,39]; in the second case, there are investigations on a charged particle-magnetic monopole scattering [40], on the quantum harmonic oscillator [41], on a quantum particle subjected to the quark–antiquark interaction [42], thermodynamic properties of a quantum particle confined in spherical box [43], and on a diatomic molecule under effects of Hulthén potential [44,45].

An elastic medium defined by the presence of a phase discontinuity (PD) is effectively described by the following length element[22]:

$$dl^2 = \frac{dr^2}{\alpha^2} + r^2(d\theta^2 + \sin^2\theta d\varphi^2), \tag{3}$$

with $0 \leq r < \infty$, $0 \leq \theta \leq \pi$, $0 \leq \varphi \leq 2\pi$, and α is the parameter associated to the PD. If $0 < \alpha < 1$, we have an impurity; if $\alpha > 1$, we have a vacancy [22,24].

Therefore, following the steps given in Refs. [21,22], Equation (1) can be applied in the environment defined by Equation (3) in the following form:

$$\frac{\partial^2\Psi}{\partial r^2} + \frac{2}{r}\frac{\partial\Psi}{\partial r} + \frac{1}{\alpha^2 r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Psi - \frac{2mV}{\alpha^2\hbar^2}\Psi = -\frac{2mi}{\alpha^2\hbar}\frac{\partial\Psi}{\partial t}. \tag{4}$$

We can impose the separation of variables method to solve Equation (4) through the ansatz defined in the form [21,22]:

$$\Psi(r, \theta, \varphi, t) = R(r)Y_{l,m}(\theta, \varphi)e^{-Et/\hbar}, \tag{5}$$

where $R(r)$ is the radial wave function, E represents the molecule energy, and $Y_{l,m_l}(\theta, \varphi)$ are the spherical harmonics, in terms of the quantum numbers $l = 0, 1, 2, \ldots$ and

$m_l = 0, \pm 1, \pm 2, \ldots$. Therefore, by substituting Equation (5) into Equation (4), we obtain the following:

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{2m}{\alpha^2\hbar^2}\left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]R + \frac{2mE}{\alpha^2\hbar^2}R = 0, \tag{6}$$

where we have adopted the definition $\hat{L}^2 Y_{l,m_l}(\theta,\varphi) = -l(l+1)Y_{l,m_l}(\theta,\varphi)$.

Equation (6) is the radial Schrödinger equation in an environment with a PD. We can note the influence of the background on the quantum dynamics of the molecule (or particle) due to the presence of the parameter α in the structure of the differential equation, that is, $V_{\text{eff}}(r) = \frac{1}{\alpha}\left[V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right]$ and $m_{\text{eff}} = \frac{m}{\alpha^2}$. We can see that, if the defect is an impurity, both the effective potential and the mass of the molecule increase; if the parameter represents a vacancy, the mass and the effective potential of the system decrease. By making $\alpha \to 1$, we recover the radial Schrödinger equation in a flat medium (without defect).

3. Lennard-Jones Oscillations

It is well known that any potential energy, $V = V(r)$, which has a minimum point (or stability point), $r = r_0$, when subjected to a Taylor series expansion, the third term of this expansion, calculated around this stability point, behaves as a harmonic oscillator energy [21,22,46]. Mathematically, this regime, known as small oscillations, is defined as follows:

$$\left.\frac{dV(r)}{dr}\right|_{r=r_0} = 0; \quad \left.\frac{d^2V(r)}{dr^2}\right|_{r=r_0} > 0. \tag{7}$$

In Ref. [21], one of us investigated the Mie-type potential [2] to analyze a particular case of it, known as the Kratzer–Fues potential [4,5], in the small-oscillation regime. The Mie-type potential is one of the most general cases for describing the quantum dynamics of a diatomic molecule. Through it, we were able to recover potential energies such as the one mentioned above and its subcases. The Mie-type potential is defined in the following form [3]:

$$V(r) = \frac{V_0}{(a-b)}\left[b\left(\frac{r_0}{r}\right)^a - a\left(\frac{r_0}{r}\right)^b\right], \tag{8}$$

where V_0 is the dissociation energy of diatomic molecule, and $a > b > 0$. The most suitable values of a and b for inert gases and some molecules were set to $b = 6$, corresponding to the theoretical value for van der Waals forces, and a value of 9 to 12 for the parameter a. For the diatomic systems, such as gases found in atmospheric air, H_2, N_2, O_2, and CO, and in noble gases, He_2, Ne_2, and Ar_2, the best fitted value for the parameter a was 12 [47].

Another energy that can be recovered through the Mie-type potential is the LJP (V_{LJ}), which is the most widely used for diatomic systems in general. To obtain the LJP, set $a = 12$ and $b = 6$ in the Mie-type potential, that is,

$$V_{LJ} = \frac{V_0}{6}\left[6\left(\frac{r_0}{r}\right)^{12} - 12\left(\frac{r_0}{r}\right)^6\right], \tag{9}$$

where $V(r_0) = -V_0$.

Expanding the LJP in Taylor series, taking into account the conditions given in Equation (7), we obtain

$$V_{LJ}(r) = -V_0 + \frac{1}{2}\left.\frac{d^2V(r)}{dr^2}\right|_{r=r_0}(r-r_0)^2 + \mathcal{O}[(r-r_0)^c], \tag{10}$$

with $\mathcal{O}[(r-r_0)^c]$ representing terms of order $(r-r_0)^c$, with $c \geq 3$. Through this expansion, it is possible to obtain the Fermi–Pasta–Ulam (FPU) potential [48], which is defined up to the fourth-order term in $r - r_0$. Because of its simple algebraic form, the model is computationally very convenient. Two important particular cases arise from FPU potential: the quadratic plus cubic and quadratic plus quartic potentials, which, for historical reasons, are called the FPU-α and FPU-β models, respectively. Since $r - r_0$ is small, we can neglect the terms $\mathcal{O}(r-r_0)^c$. Therefore, Equation (10) is rewritten in the following form:

$$V_{LJ} \approx \frac{36V_0}{r_0^2}r^2 - \frac{72V_0}{r_0}r + 35V_0. \tag{11}$$

Equation (11) represents LJP in small oscillations regime around r_0. We have, as expected, an oscillator-like term (first term). In addition, a linear term appears, which serves to maintain the cohesion of the atoms within the diatomic molecule. We can note a stark difference between the potential obtained after expansion and the LJP. In the first case, we have an oscillator-like potential plus a linear potential, a particular case of the quark–antiquark interaction [49], to which a Coulomb term is added.

4. Diatomic Molecule Under Effects of Lennard-Jones Oscillations in an Elastic Medium

Our objective is to rigorously analyze the quantum dynamics of a non-relativistic particle influenced by LJP effects within a medium characterized by a PD, particularly in scenarios involving small oscillations. To achieve this, we will implement substitutions that enhance our understanding of these phenomena.

Thus, by substituting Equation (11) into Equation (6), we have

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} - \frac{72mV_0}{\alpha^2\hbar^2 r_0^2}r^2R + \frac{144mV_0}{\alpha^2\hbar^2 r_0}rR - \frac{70mV_0}{\alpha^2\hbar^2}R - \frac{l(l+1)}{\alpha^2 r^2}R + \frac{2mE}{\alpha^2\hbar^2}R = 0. \tag{12}$$

Let us now change the dependent variable through $R(r) = f(r)/\sqrt{r}$ into Equation (12), that is,

$$\frac{d^2f}{dr^2} + \frac{1}{r}\frac{df}{dr} + \frac{[4l(l+1)+\alpha^2]}{4\alpha^2 r^2}f - \frac{72mV_0}{\alpha^2\hbar^2 r_0^2}r^2 f + \frac{144mV_0}{\alpha^2\hbar^2 r_0}rf - \frac{70mV_0}{\alpha^2\hbar^2}f + \frac{2mE}{\alpha^2\hbar^2}f = 0 \tag{13}$$

Let us consider the change of independent variable

$$u = \frac{(72mV_0)^{1/4}}{\sqrt{\alpha\hbar r_0}}r \tag{14}$$

such that Equation (13) becomes

$$\frac{d^2f}{du^2} + \frac{1}{u}\frac{df}{du} + \frac{\gamma^2}{u^2}f - u^2 f + \beta u f + \delta f = 0, \tag{15}$$

where we define the parameters

$$\beta = 2\sqrt{\frac{r_0}{\alpha\hbar}}(72mV_0)^{1/4}; \quad \gamma^2 = \frac{4l(l+1)+\alpha^2}{4\alpha^2}; \quad \delta = \frac{r_0}{3\alpha\hbar}\sqrt{\frac{m}{2V_0}}(E - 35V_0). \tag{16}$$

Analyzing the asymptotic behavior of the differential equation given in Equation (16), imposing that its solution is well behaved (finite and continuous) at $u \to 0$ ($r \to 0$) and $u \to \infty$ ($r \to \infty$), we find the following solution in terms of the unknown function $g = g(u)$:

$$f(u) = u^{|\gamma|} e^{-\frac{1}{2}u(u-\beta)} g(u). \tag{17}$$

Therefore, by substituting Equation (17) into Equation (16), we obtain

$$\frac{d^2g}{du^2} + \left[\frac{(2|\gamma|+1)}{u} - 2u + \beta\right]\frac{dg}{du} + \left[\mu + \frac{\nu}{u}\right]g = 0, \tag{18}$$

with

$$\mu = \delta - 2(|\gamma|+1) + \frac{\beta^2}{4}; \quad \nu = \frac{\beta}{2}(2|\gamma|+1). \tag{19}$$

Equation (18) is the biconfluent Heun differential equation [50], and its solution is the biconfluent Heun function [50,51]:

$$g(u) = H_B\left(2|\gamma|, \beta, \delta + \frac{\beta^2}{4}, 0; u\right). \tag{20}$$

Equation (18) has two singular points, the origin and infinity [50]. The first is a regular singular point, while the second is an irregular singular point. Thus, we can impose a power series solution around the origin using the Fröbenius method [52],

$$g(u) = \sum_0^\infty d_j u^j. \tag{21}$$

Thus, by substituting Equation (21) into Equation (18), we obtain recurrence relation

$$d_{j+2} = \frac{-[\nu + \beta(j+1)]d_{j+1} - (\mu - 2j)d_j}{(j+2)(j+2+2|\gamma|)} \tag{22}$$

and the coefficients

$$\begin{aligned} d_1 &= -\frac{\beta}{2}d_0; \\ d_2 &= \frac{d_0}{4(1+|\gamma|)}\left[\frac{(\nu+\beta)\beta}{2} - \mu\right]. \end{aligned} \tag{23}$$

Our interest is to determine solutions of bound states. To do this, we need to truncate the biconfluent Heun series, transforming the series into polynomials of finite degree n. This is possible, in our case, if we have both truncation conditions simultaneously:

$$d_{n+1} = 0; \quad \mu = 2n, \tag{24}$$

with $n = 1, 2, 3, \ldots$. From condition $\mu = 2n$, we obtain the expression

$$E_{l,n} = 71V_0 + \frac{6\alpha\hbar}{r_0}\sqrt{\frac{2V_0}{m}}(1 + n + |\gamma|). \tag{25}$$

Although the expression given in Equation (25) seems to correspond to the energy levels of the system, this is not true; it is a necessary expression to obtain the non-relativistic energy levels of the system. It is worth remembering that it is necessary to simultaneously use the two truncation conditions of the biconfluent Heun series given in Equation (24). This is only possible by assigning values to the radial modes. Thus, consider $n = 1$, which represents the radial mode that represents the lowest energy state of the quantum system. That is, setting $n = 1$ under the conditions given in Equation (24), we obtain the following mathematical expressions:

$$d_2 = 0; \quad \mu = 2, \tag{26}$$

where the condition $\mu = 2$ give us the expression

$$E_{l,1} = 71V_0 + \frac{6\alpha\hbar}{r_0}\sqrt{\frac{2V_0}{m}}(2 + |\gamma|). \tag{27}$$

The expression $d_2 = 0$ requires us to choose a fitting parameter to provide physical meaning, not only for $n = 1$ but also for any radial mode. Thus, based on the hydrogen atom problem [46] and other recent results [22,37], we consider the radial point that represents the stability point of the LJP, r_0. This allows us to obtain a feasible physical result not only for the $d_2 = 0$ condition, but also for the $d_{n+1} = 0$ condition for any value of n; $d_2 = 0$ gives us

$$\frac{1}{r_0^{l,1}} = \frac{(E_{l,1} - 35V_0)}{6\alpha\hbar(|\gamma| + 1)}\sqrt{\frac{m}{2V_0}} - 6\frac{\sqrt{2mV_0}}{\alpha\hbar}. \tag{28}$$

We can note that r_0 depends of $E_{l,1}$ for $n = 1$. Then, for any n, r_0 depends of $E_{l,n}$. In addition, r_0 also depends of γ, that is, of l and α. Therefore, we can rewrite r_0 in form $r_0 = r_0^{l,n}$. Taking this fact into consideration, we can rewrite the condition given in Equation (25) as follows:

$$E_{l,n} = 71V_0 + \frac{6\alpha\hbar}{r_0^{l,n}}\sqrt{\frac{2V_0}{m}}(1 + n + |\gamma|). \tag{29}$$

Therefore, for our analysis of the construction of the first degree biconfluent Heun polynomial to become complete, consider $n = 1$ in Equation (29) and then replace Equation (28) in it, from which we obtain

$$E_{l,1} = 36V_0(|\gamma| + 1)(2|\gamma| + 3). \tag{30}$$

Equation (30) represents the allowed values of non-relativistic energy of the diatomic molecule in small oscillations regime of LJP in an environment with a PD (vacancy or impurity) for the ground state. We can observe that the ground state energy levels of the quantum system is influenced by the medium geometry due presence of the parameter associated to the PD, that is, $\gamma = \gamma(\alpha) \sim \frac{1}{\alpha^2}$. If the defect is an impurity $(0 < \alpha < 1)$, γ increases, and, consequently, the allowed energy values for the ground state also increase; if the defect is a vacancy $(\alpha > 1)$, then γ decreases, and, consequently, the allowed energy values for the ground state also decrease. In addition, in contrast to the problem of the quantum oscillator, the quantum number associated to the ground state is not $n = 0$ [41,42], but $n = 1$. By making $\alpha \to 1$ in Equation (30), we recover the allowed values of non-relativistic energy of the diatomic molecule in the small oscillations regime of LJP in a flat medium.

With Equation (30) in hand, it is possible to determine the allowed values of the stability point of the diatomic molecule when subjected to small oscillations of the LJP, that is, substituting Equation (30) into Equation (28), we have

$$r_0^{l,1} = \frac{6\sqrt{2}\alpha\hbar(|\gamma| + 1)}{\sqrt{mV_0}[36(|\gamma| + 1)(2|\gamma| + 3) - 107]}, \tag{31}$$

that is, we can see that the stability point of the diatomic molecule has also allowed values that depend of the quantum numbers $\{l, n\}$ and of PD. In addition, we can observe also that $r_0^{l,1} = r_0^{l,1}(\alpha) \sim \alpha^2$, that is, if in the medium there is an impurity, the allowed values

of the stability radial point have an increase; if in the medium there is a vacancy, then the allowed values of the stability radial point have a decrease. In the particular case where α is large, that is, $\alpha \to \infty$, it is noted that $|\gamma| \to \frac{1}{2}$; therefore $r_0^{l,1}$, in this limit, grows linearly, $r_0^{l,1} \sim \alpha$, consequently, the stability point diverges in this case. By taking $\alpha \to 1$ we recover the allowed values of the stability point of the diatomic molecule in a flat medium.

We know that, in the study of simple harmonic motion, the total energy of the system (kinetic energy plus potential energy) is given by $E = \frac{1}{2}m\omega^2 r_m^2$, with ω being the angular frequency and r_m the maximum amplitude. The results obtained in this section should be valid in the regime of small oscillations originating from the LJP. Therefore, the regime of small oscillations of the LJP is valid in the interval $r_m = \pm\frac{1}{\omega_{LJ}}\sqrt{\frac{2E}{m}}$, where $\omega_{LJ} = \frac{6}{r_0}\sqrt{\frac{2V_0}{m}}$ is the angular frequency of Lennard-Jones, which, for the lowest energy state, as defined in Equations (30) and (31), the radial range of validity of small oscillations becomes $r_m = \pm\frac{r_0^{l,1}}{6}\sqrt{\frac{E_{l,1}}{V_0}}$.

5. Conclusions

We have investigated a diatomic molecule subjected to the small oscillations of LJP in an elastic environment defined by the presence of a PD, which can be an impurity or a vacancy. In our purely analytical analysis, searching for solutions of bound state, we defined the system energy profile and were able to observe some differences from the standard harmonic oscillator problem. We noted that the energy levels are not defined by a single, closed mathematical expression, as occurs in the quantum harmonic oscillator with spherical symmetry. Another difference from the standard problem is that the quantum number associated with the lowest energy state is not described by the radial mode $n = 0$, but rather by the radial mode $n = 1$; the principal quantum number starts at one. Furthermore, another quantum effect can be observed: the radial stability point of the LJP is quantized, that is, it depends on the system quantum numbers.

For the lowest energy state of the system, we find the allowed values of energy and the radial stability point of the LJP. In the case of the allowed energy values, we show that they depend on the PD, which can be increased or decreased if the PD represents an impurity or a vacancy, respectively. As for the radial stability point of the LJP, the influence of the PD on them is either increasing or decreasing if the PD represents vacancy or impurity, respectively. In both results found, by taking $\alpha \to 1$, we recover the particular case without defect, that is, in a medium without elasticity or flat.

As stated before, the harmonic oscillator potential is of tremendous importance in physics, as it is a prototype of any physical system involving oscillations. For example, it is used in the study of atomic vibrations in diatomic molecules, such as He_2, Ne_2, Ar_2, H_2, O_2, and CO [1]. LJP has a region around a stability point in which its interaction falls into a harmonic oscillator potential. Therefore, the results obtained in this purely analytical analysis describe systems of diatomic molecules like those mentioned above around this stability point. Our interest lies solely in the small-oscillation regime, due to the possibility of a theoretical and analytical study, and our goal is to compare it with results already well known in the academic literature, such as quantum harmonic oscillators.

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References

1. Araújo, J.P.; Ballester, M.Y. A comparative review of 50 analytical representation of potential energy interaction for diatomic systems: 100 years of history. *Int. J. Quantum Chem.* **2021**, *121*, e26808. [CrossRef]
2. Mie, G. Zur kinetischen Theorie der einatomigen Körper. *Ann. Phys.* **1903**, *316*, 657. [CrossRef]
3. Agboola, D. Complete Analytic Solutions of the Mie-type Potentials in N-Dimensions. *Acta Phys. Pol. A* **2009**, *120*, 371. [CrossRef]
4. Kratzer, A. Die ultraroten rotationsspektren der halogenwasserstoffe. *Z. Phys.* **1920**, *3*, 289. [CrossRef]
5. Fues, E. Das Eigenschwingungsspektrum zweiatomiger Moleküle in der Undulationsmechanik. *Ann. Phys.* **1926**, *80*, 367. [CrossRef]
6. Lennard-Jones, J.E. On the determination of molecular fields.II. From the equation of state of a gas. *Proc. R. Soc. Lond. A* **1924**, *106*, 463.
7. Lennard-Jones, J.E. On the determination of molecular fields.I. From the variation of the viscosity of a gas with temperature. *Proc. R. Soc. Lond. A* **1924**, *106*, 441.
8. He, Y.; Seaton, N.A. Monte Carlo simulation of the isosteric heats—Implications for the characterisation of porous materials. In *Studies in Surface Science and Catalysis*; Elsevier: Amsterdam, The Netherlands, 2007; Volume 160.
9. Cai, W.; Li, J.; Uberuaga, B.P.; Yip, S. *Comprehensive Nuclear Materials*; Elsevier: Amsterdam, The Netherlands, 2020; Volume 1.
10. Stephan, S.; Thol, M.; Vrabec, J.; Hasse, H. Thermophysical Properties of the Lennard-Jones Fluid: Database and Data Assessment. *J. Chem. Inf. Model.* **2019**, *59*, 4248. [CrossRef]
11. Fuentes-Azcatl, R.; Barbosa, M.C. Thermodynamic and dynamic anomalous behavior in the TIP4P/water model. *Physica A* **2016**, *444*, 86. [CrossRef]
12. Glotzer, S.C.; Horsch, M.A.; Iacovella, C.R.; Zhang, Z.; Chan, E.R.; Zhang, X. Self-assembly of anisotropic tethered nanoparticle shape amphiphiles. *Curr. Opin. Colloid Interface Sci.* **2005**, *10*, 287. [CrossRef]
13. Lepria, S.; Livi, R.; Politi, A. Thermal conduction in classical low-dimensional lattices. *Phys. Rep.* **2003**, *377*, 1. [CrossRef]
14. Adams, J.B. *Encyclopedia of Materials: Science and Technology*; Elsevier: Amsterdam, The Netherlands, 2001.
15. Atkins, P.; Jones, L.; Laverman, L. *Princípios de Química: Questionando a Vida Moderna e o Meio Ambiente*, 7th ed.; Bookman: Porto Alegre, Brazil, 2018.
16. Porcelli, D.; Pepin, R.O. The Origin of Noble Gases and Major Volatiles in the Terrestrial Planets. *Treatise Geochem.* **2003**, *4*, 319.
17. Frenkel, D.; Smit, B. *Understanding Molecular Simulation: From Algorithms to Applications*, 2nd ed.; Elsevier: Amsterdam, The Netherlands, 2002.
18. Chiquito, A.J.; Almeida, N.G. O Potencial de Lennard-Jones: Aplicação à Moléculas Diatômicas. *Rev. Bras. Ensino Física* **1999**, *21*, 2.
19. Pereira, L.F.C.; Silva, E.O. Modification of Landau Levels in a 2D Ring Due to Rotation Effects and Edge States. *Ann. Phys.* **2023**, *535*, 2200371. [CrossRef]
20. Marques, G.A.; Bezerra, V.B. Non-relativistic quantum systems on topological defects spacetimes. *Class. Quantum Grav.* **2002**, *19*, 985. [CrossRef]
21. Vitória, R.L.L.; da Silva, K.A.T. Effects of small oscillations on a diatomic molecule in an elastic medium. *Eur. Phys. J. Plus* **2023**, *138*, 172. [CrossRef]
22. Vitória, R.L.L.; Pereira, C.F.S.; Martins, S.M.S.B. Thermodynamic Properties of a Diatomic Molecule Under Effects of Small Oscillations in an Elastic Environment. *Symmetry* **2025**, *17*, 1038. [CrossRef]
23. Eisberg, R.M.; Resnick, R. *Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particle*, 2nd ed.; Wiley: Hoboken, NJ, USA, 1985.
24. Katanaev, M.O.; Volovich, I.V. Theory of defects in solids and three-dimensional gravity. *Ann. Phys.* **1992**, *216*, 1. [CrossRef]
25. Volterra, V. Sur léquilibre des corps élastiques multiplement connexes. *Ann. Sci. lÉcole Norm. Supérieure* **1907**, *24*, 401. [CrossRef]
26. Barriola, M.; Vilenkin, A. Gravitational field of a global monopole. *Phys. Rev. Lett.* **1989**, *63*, 341. [CrossRef]
27. Vilenkin, A.; Shellard, E.P.S. *Strings and Other Topological Defects*; Cambrigde University Press: Cambridge, UK, 1994.
28. de Mello, E.R.B. Physics in the global monopole spacetime. *Braz. J. Phys.* **2001**, *31*, 211. [CrossRef]
29. Caramês, T.R.P.; Fabris, J.C.; de Mello, E.R.B.; Belich, H. f(R) global monopole revisited. *Eur. Phys. J. C* **2017**, *77*, 496. [CrossRef]
30. de Mello, E.R.B.; Saharian, A.A. Scalar self-energy for a charged particle in global monopole spacetime with a spherical boundary. *Class. Quant. Gravit.* **2012**, *29*, 135007. [CrossRef]

31. de Mello, E.R.B.; Furtado, C. Nonrelativistic scattering problem by a global monopole. *Phys. Rev. D* **1997**, *56*, 1345. [CrossRef]
32. de Mello, E.R.B.; Carvalho, F.C. Vacuum polarization for a massless spin-1/2 field in the global monopole spacetime at nonzero temperature. *Class. Quant. Gravit.* **2001**, *18*, 5455.
33. de Mello, E.R.B.; Carvalho, F.C. Vacuum polarization for amassless scalar field in the global monopole spacetime at finitetemperature. *Class. Quant. Gravit.* **2001**, *18*, 1637.
34. Boumali, A.; Aounallah, H. Exact Solutions of Scalar Bosons in the Presence of the Aharonov-Bohm and Coulomb Potentials in the Gravitational Field of Topological Defects. *Adv. High Energy Phys.* **2018**, *2018*, 1031763. [CrossRef]
35. de Oliveira, A.L.C.; de Mello, E.R.B. Exact solutions of the Klein Gordon equation in the presence of a dyon, magnetic flux and scalar potential in the spacetime of gravitational defects. *Class. Quant. Gravit.* **2006**, *23*, 5249. [CrossRef]
36. Bragança, E.A.F.; Vitória, R.L.L.; Belich, H.; de Mello, E.R.B. Relativistic quantum oscillators in the global monopole spacetime. *Eur. Phys. J. C* **2020**, *80*, 206. [CrossRef]
37. Vitória, R.L.L.; da Silva, K.A.T. Hydrogen and Pionic Atoms Under the Effects of Oscillations in the Global Monopole Spacetime. *Symmetry* **2025**, *17*, 88. [CrossRef]
38. Aounallah, H.; Soares, A.R.; Vitória, R.L.L. Scalar field and deflection of light under the effects of topologically charged Ellis-Bronnikov-type wormhole spacetime. *Eur. Phys. J. C* **2020**, *80*, 447. [CrossRef]
39. Soares, A.R.; Vitória, R.L.L.; Aounallah, H. On the Klein-Gordon oscillator in topologically charged Ellis–Bronnikov-type wormhole spacetime. *Eur. Phys. J. Plus* **2021**, *136*, 966. [CrossRef]
40. Cavalcanti de Oliveira, A.L.; de Mello, E.R.B. Nonrelativistic charged particle-magnetic monopole scattering in the global monopole background. *Int. J. Mod. Phys. A* **2003**, *18*, 3175. [CrossRef]
41. Furtado, C.; Moraes, F. Harmonic oscillator interacting with conical singularities. *J. Phys. A Math. Gen.* **2000**, *33*, 5513. [CrossRef]
42. Vitória, R.L.L.; Belich, H. Harmonic oscillator in an environment with a pointlike defect. *Phys. Scr.* **2019**, *94*, 125301. [CrossRef]
43. Vitória, R.L.L.; Moy, T.; Belich, H. Thermodynamics Properties of a Quantum Particle Confined into Two Elastic Concentric Spheres. *Few-Body Syst.* **2022**, *63*, 51. [CrossRef]
44. Bakke, K. Topological effects of a global monopole on the Hulthén potential. *Eur. Phys. J. Plus* **2023**, *138*, 85. [CrossRef]
45. Alves, S.S.; Cunha, M.M.; Hassanabadi, H.; Silva, E.O. Approximate Analytical Solutions of the Schrödinger Equation with Hulthén Potential in the Global Monopole Spacetime. *Universe* **2023**, *9*, 132. [CrossRef]
46. Griffiths, J.D. *Introduction to the Quantum Mechanics*; Prentice Hall: Upper Saddle River, NJ, USA, 1995.
47. Lennard-Jones, J.E. The equation of state of gases and critical phenomena. *Physica* **1937**, *4*, 941. [CrossRef]
48. Fermi, E.; Pasta, J.; Ulam, S. *Collected Papers*; Fermi, E., Ed.; University of Chicago Press: Chicago, IL, USA, 1965; Volume 2, p. 78.
49. Bahar, M.K.; Yasuk, F. Exact Solutions of the Mass-Dependent Klein-Gordon Equation with the Vector Quark-Antiquark Interaction and Harmonic Oscillator Potential. *Adv. High Energy Phys.* **2013**, *2013*, 814985. [CrossRef]
50. Ronveaux, A. *Heun's Differential Equations*; Oxford University Press: Oxford, UK, 1995.
51. Medeiros, E.R.F.; de Mello, E.R.B. Relativistic quantum dynamics of a charged particle in cosmic string spacetime in the presence of magnetic field and scalar potential. *Eur. Phys. J. C* **2012**, *72*, 2051. [CrossRef]
52. Arfken, G.B.; Weber, H.J. *Mathematical Methods for Physicists*, 6th ed.; Elsevier Academic Press: New York, NY, USA, 2005.

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