# Mathematical Description of Energies of Oscillating Atoms

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**Abstract -** *This research explores atomic vibrations using the Lennard-Jones Potential (LJP) to model the balance of attractive and repulsive forces between atoms. Focusing on energy exchange between kinetic and potential forms, we examine how atoms oscillate around equilibrium points. By applying these principles to hydrogen gas, we calculate energy distributions and investigate how atomic vibrations affect material properties like thermal and electrical conductivity. The study provides a theoretical foundation for understanding atomic behavior, with potential applications in materials science and thermodynamics. Limitations of the LJP are noted, such as its neglect of multi-body interactions.*

## 1.INTRODUCTION

Everything in the world around us is due to the effect of two main types of forces, the Gravitational and the Electromagnetic force. The macroscopic world works mainly on the principles of the gravitational force. However, in the microscopic world, everything is governed by electromagnetic forces that dictate the behavior of atoms and molecules, ultimately shaping the properties of matter. One of the fundamental concepts in understanding these forces is the Lennard-Jones Potential (LJP), which models the interaction between a pair of neutral atoms or molecules. The LJP describes how the potential energy between two particles changes with respect to the separation and how the electric force transitions from being attractive at longer distances to repulsive as they approach each other, preventing them from occupying the same space. This interconnection between potential energy and force can be explained by a simple mathematical equation that shows that the force exerted is the negative gradient of the potential energy distance graph. The Lennard-Jones Potential uses the parameters of the well depth and the zero of the function to describe how the Electric Potential Energy of two atoms in a bond changes with respect to the distance between the two atoms. The Lennard-Jones Equation is as follows: [1]

$$v(r) = 4\epsilon((\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6)$$

Where : V(r) represents the Electric Potential Energy when separation is r $\epsilon$ represents the Binding Strength of the Particular Bond $\sigma$ represents the Zero of the function. Since the $\sigma$ and $\epsilon$ are unique characters, the relationship between
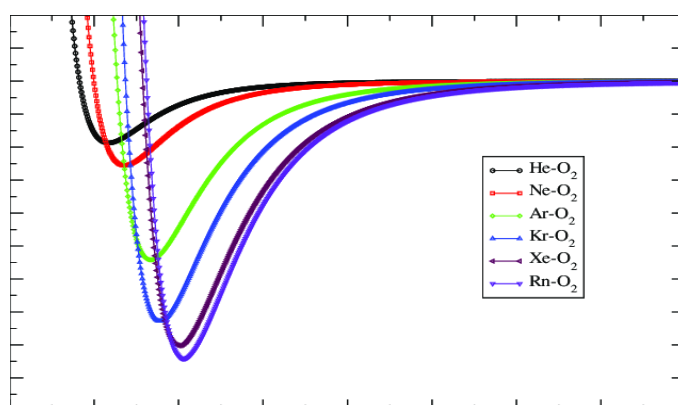


**Fig -1**: Diagram showing how the LJP graphs are different for different bonds

the Electric Potential Energy and the distance is unique to each bond. The forces acting on the atoms partaking in the bond will also be bond-specific, resulting in a certain aspect of peculiarity. The interplay of forces between the atoms, represented by the Lennard-Jones Potential equation, leads to an equilibrium state where the net force between particles is zero. Oscillations around this equilibrium position play a crucial role in determining the properties of substances. Understanding these oscillations is essential as they underlie several important phenomena including spectroscopic signatures, thermal and electrical conductivity, and reaction kinetics. This research aims to delve deeper into the oscillatory behavior of atoms as they transition between attractive and repulsive forces. We explore the energy distribution within these oscillating systems, considering the exchange between kinetic and potential energy as atoms vibrate around their equilibrium positions. By developing mathematical models and differential equations, we seek to describe these energy fluctuations and their impact on the overall behavior of materials. Through this investigation, we aim to provide a more comprehensive understanding of the internal energy in microscopic systems, offering insights into how energy is conserved and distributed at the atomic level. This research contributes to the theoretical understanding of molecular interactions and has potential

applications in fields such as material science, thermodynamics, and quantum mechanics.
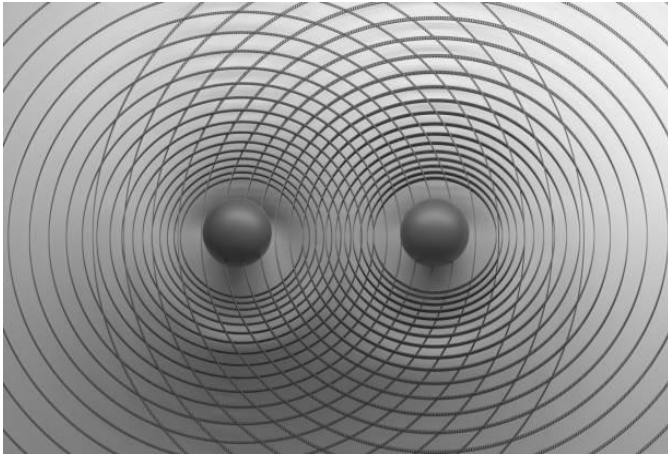
## 2.Context



**Fig - 2** : Interaction between atoms and their magnetic fields

## 2.1 Understanding the oscillation

One way of explaining the reason behind the oscillation of these atoms is electromagnetism. Since these atoms have charges and are in a constant state of motion, they can be thought of as having their own magnetic flux around them. When a nearby atom experiences any movement, it disturbs the magnetic flux of the other atoms. This disturbance of magnetic flux is what causes a force to act on the atoms such that the force opposes the cause of the disturbance, as stated by Lenz Law. This force acts as the restoring force for the oscillation. The motion of the charged particles in the magnetic field can affect the system in many different ways and the continuous change of the magnetic flux at all points between the atoms can also cause many effects. This can further be studied when the system is looked at from a quantum-mechanical point of view.

We claim that the potential graph should not be a continuous function and should instead be discrete as energy is transferred in packets (photons). It is important to study the effect of this as it can help us determine and prove that this system of atoms should be studied from a quantum-mechanical standpoint and not classical physics.

## 2.2 Understanding the Lennard Jones Potential Graph

The Lennard-Jones Potential equation shows how the potential energy of two atoms changes with respect to their separation by taking into account multiple factors and formulating the σ and ϵ of the bond. This equation

when plotted on a graph results in a 'dip'-like curve whose minimum point is at a distance of ϵ from the Y-axis and the first zero of the graph is at a distance of σ from the X-axis.
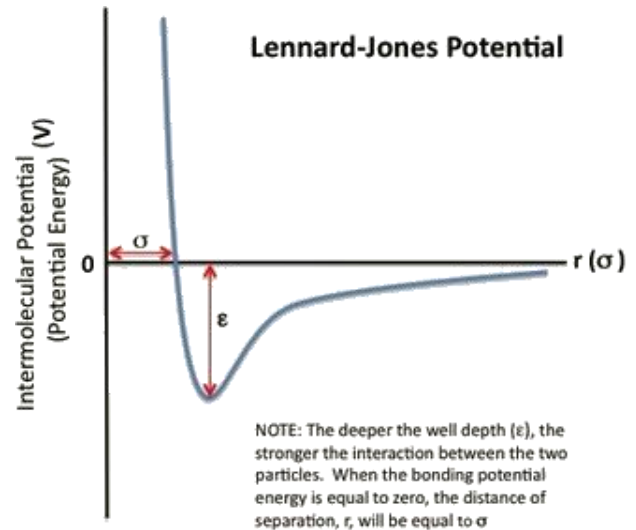


**Fig - 3** : Diagram showing the representation of σ and ϵ on the graph

Since

$$F = -\frac{\partial U}{\partial x}$$

and the minimum points are all turning points, the gradient at that point must be 0, and hence the force at the minimum point is 0 and the system is in a state of equilibrium at the minimum point. The graph can be broken into two sections at the equilibrium point. The leftward section shows repulsion as, when solved using Equation(2) the force value is negative which represents repulsion. Hence, the rightward section would show a state of attraction. We can see that the curvature of the dip is not symmetrical on both sides which shows that the strength of attraction and repulsion is not the same.

$$v(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

Repulsive Region (r < σ): Steep rise with large positive curvature, reflecting strong repulsive forces. Attractive Region (r > σ): Gentle dip with smooth curvature, as the potential gradually approaches zero. Analytically, curvature is determined using the second derivative of the potential. Hence, by finding the second derivative of the Lennard-Jones Potential Equation, we can find the analytical description of the curvature. The synthetic description highlights the sharp bend in repulsion versus the smooth transition in attraction. This would result in an asymmetrical Kinetic energy graph later on.

## 2. 3 Effects of crossing the Equilibrium Point

### 2.3.1 Electrical Conductivity

Crossing the equilibrium distance during atomic vibrations primarily affects the electrical conductivity of materials through electron-phonon interactions. When atoms move past their equilibrium positions, they create phonons that can scatter conduction electrons. Phonons are quasi-particles representing quantized vibrations of atoms in a solid lattice. They play a key role in understanding heat and sound propagation in materials. Phonon scattering increases with larger deviations from equilibrium, typically reducing the material's electrical conductivity, especially at higher temperatures where atomic vibrations are more intense. The overall effect depends on the material's structure and how strongly electron movement is coupled with atomic vibrations.

### 2.3.2 Thermal Conductivity

The phonon scattering, as mentioned above, significantly affects the thermal conductivity of a substance. This scattering can either increase or decrease thermal conductivity depending on the material. In most materials, more phonon scattering generally reduces thermal conductivity, especially at higher temperatures. However, it may increase thermal conductivity in certain polymers and complex crystalline materials under specific conditions through a process called phonon localization. The group velocity of phonons plays a key role in thermal conductivity.

$$v_g = \frac{\partial \omega}{\partial q}$$

Where ω is the angular frequency of the phonon and q is the wave factor In solids, heat is primarily conducted by phonons. Faster phonon group velocities result in more efficient energy transfer, thus enhancing the material's ability to conduct heat. This can be grouped as transport phenomena for heat and electricity and the effect of crossing the equilibrium point can be further studied. By understanding the distribution of the energies at each stage of the oscillation, we can better understand the factors that may affect phonon scattering and hence affect this transport phenomenon. In essence, this research directly helps us better interpret, understand, and manipulate phonon scattering and hence, thermal and electrical conductivity as well.

## 2.4 Limitations of the Lennard-Jones Potential Equation

One major drawback is its oversimplification of molecular interactions, as it only accounts for two-body interactions and neglects more complex multi-body interactions that can be significant in real systems. Additionally, the potential cannot describe directional bonding, such as hydrogen bonds or covalent bonds, which are crucial for many molecular structures and interactions. Another limitation is the absence of electronic polarization effects, which can influence interactions in more complex or polarizable systems.[2]

The Lennard-Jones potential is primarily applicable to noble gases and simple non-bonded interactions, making it inadequate for describing covalent, ionic, or metallic bonds. Furthermore, the parameters ε and σ in the Lennard-Jones equation are typically obtained from empirical data and may not accurately capture the nuances of interactions in different environments or under varying conditions. In high-density systems, where atoms or molecules are very close together, the potential may fail to accurately predict the repulsive forces due to its limited form. This is because other forms of attraction and repulsion such as ID-ID and PD-PD attraction are more prevalent in these systems. Moreover, the potential does not directly incorporate the effects of temperature and pressure, which can be significant in real-world scenarios. The repulsive term, with its power of 12, provides a steep increase in potential energy that might not always represent true physical behavior at very short ranges. These limitations highlight that while the Lennard-Jones potential is a useful approximation, more complex models and potentials are often necessary to accurately describe molecular interactions in many systems.

## 3. Assumptions

### 3.0.1 Comparison

The system of two atoms interacting with each other can be envisioned as a system of two blocks connected together via a spring. This comparison would imply that the oscillating atom system follows a simple harmonic motion.
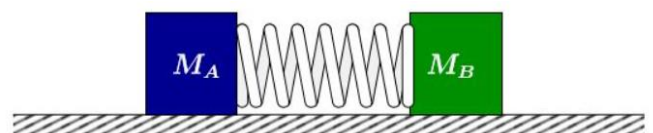


**Fig - 4** Representation of how the described 2-block system would look

The point where the spring is most compressed (maximum Elastic Potential Energy) and both the blocks are at rest would be similar to the point when the Electric Potential Energy is maximum. Following this assumption, we can say that the atomic system would follow all the equations of simple harmonic motion. This would also

mean that the distribution of potential and kinetic energy in the atomic system would be similar to that of a simple harmonic system. Hence, the atomic system would follow the following equations:

$$x = x_0 \sin(\omega t)$$

$$v = x_0\, \omega \cos(\omega t)$$

$$a = -\omega^2 x_0 \sin(\omega t) = -\omega^2 x$$

The velocity-time function shows that the velocity would be maximum when the body, atom here, is in the equilibrium position, and as the body approaches either of the ends, its velocity decreases and eventually becomes 0 at the ends. Since Kinetic energy is directly proportional to the square of velocity,

$$KE = \frac{1}{2} m v^2$$

The Kinetic energy of the system would follow a similar trend with it becoming maximum at the equilibrium point and minimum at the two end points.

$$TE = KE + PE$$

Since the Total energy is constant due to the law of conservation of energy, the Potential Energy would follow an inverse trend becoming maximum at the two end-points and minimum at the equilibrium point. Since we know that the Kinetic Energy is maximum at the equilibrium point. By assuming that the Potential Energy is α at that point, we can say that the total energy is :

$$TE = \frac{1}{2} m v_0^2 + \alpha$$

The velocity at a given point is

$$v = \omega \sqrt{x_0^2 - x^2}$$

So the maximum velocity is

$$v_0 = \omega x_0$$

Conventionally, it is assumed that the Potential energy of the system is 0 at the equilibrium point giving α the value of 0 and hence simplifying the Total Energy equation.
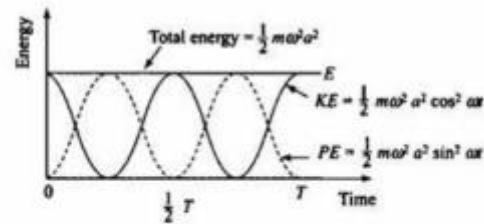


Figure 5: graph of KE and PE with respect to separation

### 3.0.2 Implications

With this in mind, we have a rough idea about the description of the kinetic and potential energies of the oscillating atoms. Figure 5 represents how the Energies of the oscillating atoms would change. Both the Energy graphs have a sinusoidal nature due to the cosine and sine functions present in the Simple Harmonic Motion equations. The total energy too is shown with its equation in a different form. We can see that the total energy is invariant to the separation. Hence abiding by the law of conservation of energy. The above graph, however, represents the energy change in a dynamic system. The total energy of a system can change due to external factors.

$$\frac{\partial E}{\partial t} = \frac{\partial}{\partial t} \frac{1}{2} m v^2 + \frac{\partial}{\partial t} \frac{1}{2} k x^2$$

$$\frac{\partial E}{\partial t} = \frac{1}{2}\left( \frac{\partial m}{\partial t} v^2 + m \frac{\partial v^2}{\partial t} \right) + \frac{1}{2}\left( \frac{\partial k}{\partial t} x^2 + k \frac{\partial x^2}{\partial t} \right)$$

$$\frac{\partial E}{\partial t} = \frac{1}{2}\left( 0 + m \frac{\partial v^2}{\partial t} \right) + \frac{1}{2}\left( 0 + k \frac{\partial x^2}{\partial t} \right)$$

$$\frac{\partial E}{\partial t} = \frac{1}{2}\left( 2mv \frac{\partial v}{\partial t} \right) + \frac{1}{2}\left( 2kx \frac{\partial x}{\partial t} \right)$$

$$\frac{\partial E}{\partial t} = mva + kxv$$

If an energy source is connected to the system, the total energy would increase with respect to time. Figure 6 is an Energy-Time graph that plots the Kinetic and Potential

energies. As shown in Figure 6, both the kinetic and potential energies would increase with time but would still retain their sinusoidal characteristics and time period. In essence, only the amplitude of the Energies has changed.
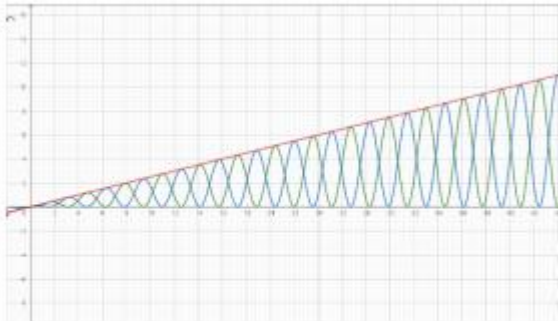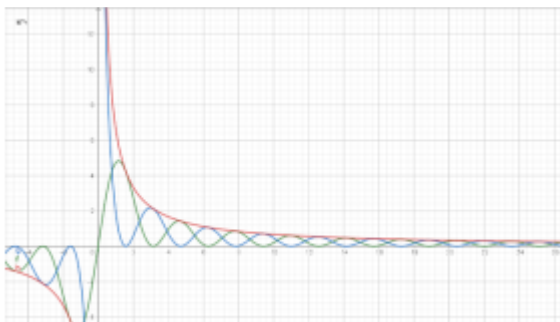


Figure 6: Increasing Total Energy

The gradient of the Total Energy graph would indicate the rate at which energy is supplied to the system by the source or the power of the energy source.



If, on the other hand, any substance that removes energy from the system is connected to the system, then the total energy would decrease with respect to time. Figure 7 is an Energy-Time graph that shows the Kinetic and Potential Energies. As shown in Figure 7, both the kinetic and potential energies would decrease over time but will still retain their characteristics. The gradient of the graph indicates the rate at which energy is removed from the system. The amplitude decreases exponentially this shows that eventually, the atoms come to an apparent state of rest where the magnitude of the displacement from the mean position is negligible. However, it is important to note that this only occurs in those systems in which energy is continuously drawn out and is not applicable in real-world scenarios.

### 3.0.3 Reality

However, it is important for us to realize that the Movement of atoms does not actually follow a Simple Harmonic Motion. This is because the atoms do not follow the most important postulate of simple harmonic motion which is, the acceleration experienced must be directly proportional to the displacement and must be in the opposite direction. This can be seen, as the Lennard-Jones Equation shows that Potential Energy has an inverse relationship with distance. Hence, when differentiated to find force, the equation would still show an inverse relationship showing that acceleration is not proportional to the negative displacement.

### 4. Computations

Hence, we have established that the oscillating atoms follow an an-harmonic oscillation. It is, however, necessary for us to find the ranges of separations that these atoms undergo to accurately formulate the functions that would describe the energies. To do this, we must find the total energy that each individual molecule would possess and move forward accordingly. We use Hydrogen gas as the sample molecule for all assumptions and calculations as it has minimum mass and its diatomic nature makes calculations easy and accurate. Initially, we approached this problem using the ideal gas energy equation. However, we later discarded this as the ideal gas equation assumes that there are no intermolecular forces of attraction or repulsion. This means it takes the potential energy to be 0 at all times which directly contradicts the Lennard-Jones Potential Equation.

$$E = \frac{5}{2}K_B T$$

Where $K_B$ stands for Boltzmann constant and T stands for Thermodynamic Temperature. 5/2 is used as the hydrogen gas will have 5 degrees of freedom as it is a diatomic gas.

We then decided to use enthalpy change as a measure of finding the energy possessed by a singular molecule. The actual amount of the internal energy can never be found but the change in energy can be found. We can estimate the energy possessed by finding the enthalpy change of the gas from 0K (absolute zero) to any particular temperature(273K in this case).

However, the specific heat capacity of a substance is not constant and changes depending on the temperature. We assume that the specific heat capacity remains unchanged throughout the calculation and the value is similar to the specific heat capacity at room temp. By taking the value of c to be 14.20JK−1g −1, we find that the energy possessed by each molecule of hydrogen gas is $1.30 * 10{-20}$. This energy is then distributed between the kinetic and potential energies. For the scope of this research paper, we will represent all the parameters as symbols instead of their actual values. Substituting the real data values in the equation to find an accurate numerical result may be done later.[3]

$$Q = mc\Delta T$$

$$Q = mc(273 - 0)$$

$$Energy\ per\ molecule = \frac{273mc}{n\ N_A}$$

$$= \frac{m}{n} \times \frac{273c}{N_A}$$

$$= \frac{273c \times Mr}{6.02 \times 10^{23}}$$

$$= \frac{2 \times 273 \times c}{6.02 \times 10^{23}}$$

IrjBy plotting the Total Energy of a molecule on the same graph as the Lennard Jones Potential, it is possible for us to find the points of separation at which the Potential Energy is maximum and hence Kinetic Energy is 0. These points would serve as the endpoints of the oscillation as the velocity is 0 meaning that the atoms are changing their direction of motion.
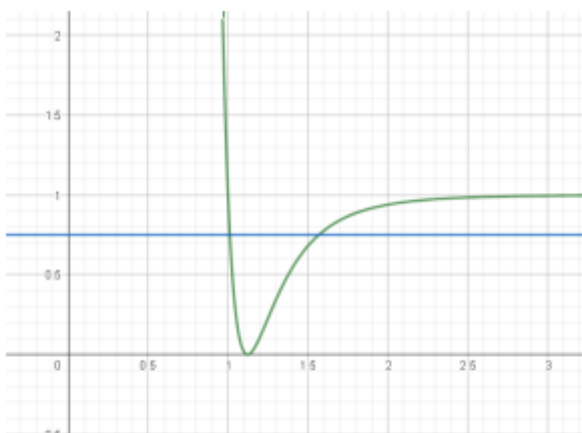


Figure 9: Diagram showing how the Total Energy and LJP can be plotted

Figure 9 is a Energy-Separation graph which shows the Total Energy and Potential Energy. Figure 9 shows how the Total Energy and the Potential Energy of these oscillating atoms would be represented. The X coordinates of the points of intersection of the 2 graphs show the range within which the separation of the atoms is allowed to exist. By using the Total Energy Equation $T\ E = KE + P\ E$, we know that the Kinetic Energy will be the positive difference between the Total Energy and Potential Energy graphs. Figure 10, an Energy-Separation plot, shows the Kinetic Energy(Red), Potential Energy(Green), and Total Energy(Blue) possessed by a single hydrogen molecule.
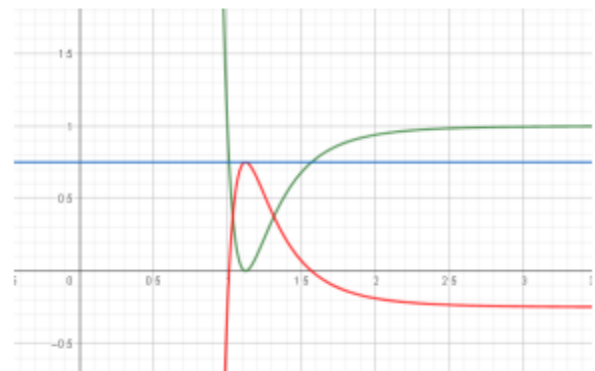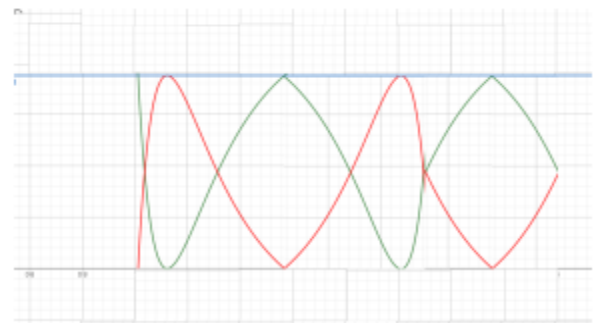


Figure 10: Diagram showing all the Energies possessed



Figure 11: Energy-Time graph of oscillating atoms

## 5. CONCLUSION

In conclusion, we can determine that the Energies of a system of oscillating atoms change dynamically in a set pattern and this pattern is influenced by the Lennard-Jones Potential of the bond. This research explores the oscillatory behavior of atoms as described by the Lennard-Jones Potential (LJP), providing insights into how potential and kinetic energy fluctuate during atomic interactions. By modeling these interactions and comparing them to simple harmonic motion, we observed that while the oscillations of atoms share similarities with classical harmonic systems, they are inherently anharmonic due to the nature of molecular forces. The Lennard-Jones Potential effectively describes the interactions between neutral atoms, demonstrating how electric potential energy changes with separation. Our analysis of energy distribution reveals how atoms transition between attractive and repulsive forces, oscillating around an equilibrium point where the net force is zero. These oscillations influence key material properties such as thermal and electrical conductivity, as deviations from equilibrium lead to phonon scattering. We also acknowledge the limitations of the Lennard-Jones

Potential, particularly in its oversimplification of molecular interactions and its inability to account for multi-body interactions, directional bonding, and electronic polarization. Despite these limitations, the LJP remains a valuable tool for understanding fundamental molecular behavior, especially in simple systems like noble gases. By developing mathematical models and computing energy distributions for hydrogen gas, we have established a framework for studying atomic vibrations and their implications for material properties. Future research could focus on addressing the limitations of the Lennard-Jones Potential by incorporating more complex interactions, temperature and pressure effects, and exploring its applicability to a broader range of materials and molecular structures. This work contributes to a deeper theoretical understanding of atomic oscillations and their role in determining the behavior of substances in various scientific and engineering contexts.

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| $\epsilon$ | Binding Strength of the Bond |
| $\sigma$ | 1st Zero of the LJP graph |
| U | Potential Energy |
| x | Displacement |
| $\omega$ | Angular Frequency of the Phonon |
| q | Wavefactor |
| v | Velocity |
| a | Acceleration |
| $x_0$ | Amplitude |
| t | Time |
| m | Mass |
| k | Spring Constant |
| $K_B$ | Boltzmann's Constant |
| T | Thermodynamic Temperature |
| Q | Energy gained |
| c | Specific Heat Capacity |
| n | Number of Moles |
| $N_A$ | Avogaro's Constant |
| Mr | Molecular Mass Ratio |