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The Morse Oscillator's Free Motion as the One-Dimensional Analogue for the Kepler Problem

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ABSTRACT

We obtained the expressions for Morse oscillator classical motion with explicit dependence on initial coordinate and velocity. These formulas provide the easy comparison with results of numerical calculations, and in addition to previous considerations, they take into account the possible different sign of initial velocity of the oscillator. The analogy between the free motion of a Morse oscillator and motion of a particle in gravitation field (i.e. the Kepler problem) is drawn up.

Keywords: Morse Potential; Morse Oscillator; Kepler Problem; Free Oscillations; Infinite Motion Pasc. 45.50.-j

Introduction

It is well known that the harmonic oscillator model can be employed for weakly excited mechanical systems. When excitation grows, anharmonicity begins to be noticeable and more sophisticated models should be used. One of these models is the Morse oscillator which is especially useful for the description of diatomic molecule oscillations. For example, the experimental value of the dimensionless the anharmonicity parameter for the CO molecule is xe = 0.00612. The anharmonicity parameter serves as a measure of the deviation of the real oscillator's discrete spectrum from the equidistant approximation. In the Morse model, xe = 0.00608, so the relative error is only 0.65%. The Morse model is mostly used in quantum mechanics. Particularly, the exact wave function of a particle in the Morse potential is well-known for many decades [1]. Classical applications of the Morse model are not so numerous. To our knowledge, the first work with the exact analytical solution for the Morse oscillator's classical motion is paper [2]. This problem was also considered 30 years later [3]. In these papers, similar expressions were obtained while using slightly different approaches. Regardless of the abovementioned articles, we have also found analytical expressions for the free motion of the Morse oscillator [4]. Our formulas were obtained using the energy conservation law without solving any differential equations. They also were written in another form when compared with the results of [2,3]. Below we introduce our consideration of the problem which provides some additions to previous results [2,3]. Moreover, we demonstrate the analogy between the free motion of a Morse oscillator and motion of a particle in a gravitation field.

Definition and Main Characteristics of a Morse Oscillator

The potential energy of Morse oscillator is given [1] by the following formula:

$$U^{(Morse)}(x) = D\left\{\exp(-2\,k\,x) - 2\exp(-k\,x)\right\}, \quad (1)$$

where D is the binding energy, k is the parameter of the potential, x is the displacement of the oscillator's coordinate from its equilibrium position. In the case of a diatomic molecule, $x = r - r_e$, where r and r_e are the current and the equilibrium distances between the nuclei, respectively. While the displacement from the equilibrium position is small, when $x < 1/k$, the Morse potential function transforms into the parabolic dependence. This relation of the potential energy on the coordinate is typical for a harmonic oscillator: $U^{(Morse)}(x) \approx D\left\{k^2\,x^2 - 1\right\}$. In Figure 1, the graph of the Morse potential energy is plotted using the parameters of a carbon monoxide (CO) molecule, together with its corresponding harmonic approximation. Comparing the graphs of the Morse potential and the harmonic potential energies, the Morse potential energy's asymmetrical shape is remarkable. This shape has the horizontal asymptote $U = 0$ as x tends to infinity, $x > 1/k$. This asymptote divides the energy spectrum of the oscillator into two parts: the positive part with $U > 0$ and the negative part with $U < 0$. The negative part of the spectrum corresponds to the oscillator's finite motion, and on the contrary, the positive part of the spectrum corresponds to the infinite motion. When the motion is infinite, the coordinate increases indefinitely, and the oscillations turn into expansion. If we use the Morse potential energy to describe a diatomic molecule, the negative part of the energy spectrum will correspond to the oscillations of the atoms forming a molecule in a limited space. The positive part of the energy spectrum in this case will correspond to the dissociated state of the molecule, in which the distance between atoms grows up to infinity. Within such model, the binding energy D receives the meaning of the molecule's dissociation energy. Hence, the Morse potential describes both the atoms oscillatory motion and their expansion.

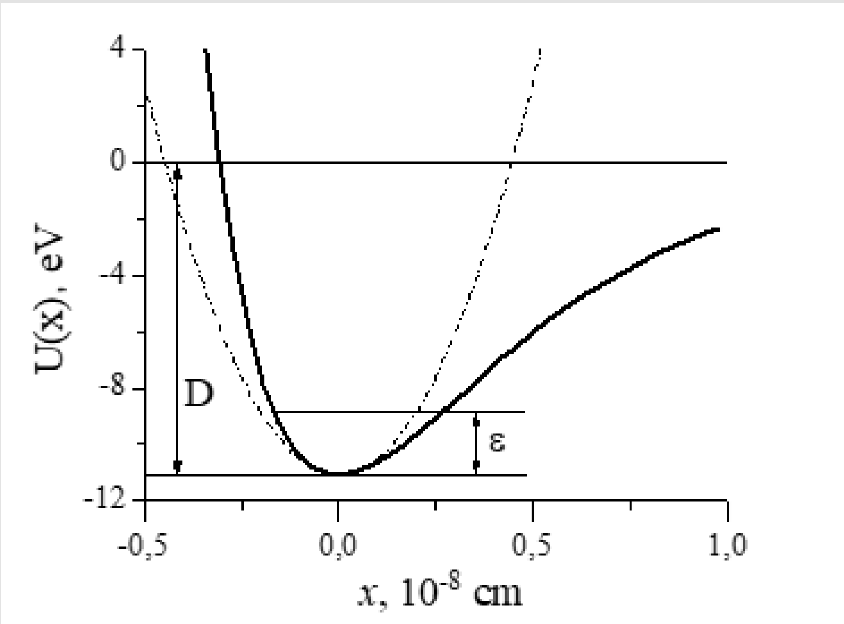

Figure 1: The Morse potential energy plotted using the parameters of a CO molecule (solid thick curve) and its corresponding harmonic approximation (dash-dotted curve).

Free Oscillations of the Morse Oscillator

Consider the free motion of a Morse oscillator for given total energy ε measured from the bottom of a potential well (Figure 1). It is convenient to introduce a dimensionless displacement of the coordinate from its equilibrium position, $y = k\,x$, and dimensionless time, $\tau = \omega_0\,t$ (ω_0 is own frequency of the oscillator in harmonic approximation). In the future, for brevity, we will call these variables simply the coordinate and time.

Using such definitions, the Morse oscillator's motion equation can be written as the following:

$$\ddot{y}_{\tau^2} = \exp(-2\,y) - \exp(-y). \quad (2)$$

Note that the dimensionless Eq. (2) does not contain the binding energy D and the parameter of the potential k, so it is universal for the given type of potential energy. To determine the

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dependence $y(\tau)$, it is convenient to use the law of conservation of energy, which in dimensionless variables can be written as the following equation:

$$\dot{y}_\tau^2 + \exp(-2y) - 2\exp(-y) = \tilde{\varepsilon} - 1, \quad (3)$$

where $\tilde{\varepsilon} = \varepsilon / D$ is dimensionless energy. Here, the first term on the left side of the equation corresponds to the kinetic energy, while the second and the third terms represent the potential energy. The solution of (3) depends on the magnitude of the dimensionless energy $\tilde{\varepsilon}$. Three cases, which correspond to three motion modes, can be differentiated: the first one, when $1 > \tilde{\varepsilon} > 0$, the second, when $\tilde{\varepsilon} = 1$, and the third, when $\tilde{\varepsilon} > 1$. Below it will be demonstrated that the first case corresponds to the finite motion, i.e., oscillations of the Morse oscillator, while the latter two cases correspond to the infinite motion, i.e., the expansion mode. For a finite movement which corresponds to the oscillatory mode, $1 > \tilde{\varepsilon} > 0$. Solving (3), the following dependence is obtained [3, 4]:

$$\tau - \tau_0 = \int_{y_0}^{y} \frac{dy'}{\sqrt{\tilde{\varepsilon} - 1 + 2\exp(-y') - \exp(-2y')}}, \quad (4)$$

where τ_0 is the integration constant (which we will later assume is zero) and $y_0 = y(\tau_0)$.

The (4) yields the dependence $y(\tau)$ in an implicit form. To obtain the explicit form of the function $y(\tau)$, the integral on the right-hand side of (4) needs to be calculated and then y needs to be expressed via the dimensionless time τ. The resulting formula is

$$y(\tau) = \ln\left\{\frac{1 - \sqrt{\tilde{\varepsilon}}\sin\left[\pm\sqrt{1-\tilde{\varepsilon}}\,\tau + \varphi(\tilde{\varepsilon}, y_0)\right]}{1 - \tilde{\varepsilon}}\right\}, \quad (5)$$

where

$$\varphi(\tilde{\varepsilon}, y_0) = \arcsin\left\{\frac{(\tilde{\varepsilon} - 1)\exp(y_0) + 1}{\sqrt{\tilde{\varepsilon}}}\right\} \quad (6)$$

is the initial phase of the oscillations dependent on initial displacement $y_0 = y(\tau = 0)$.

The sign in front of the square root depends on the sign of initial velocity of the oscillator $\dot{y}_0 = \dot{y}(\tau = 0)$.

The resulting expression is valid while the dimensionless energy $1 > \tilde{\varepsilon} > 0$. This corresponds to the negative part of the energy spectrum. The harmonic approximation is valid for low excitation energies of the Morse oscillator, i.e., for $\tilde{\varepsilon} < 1$ ($\varepsilon < D$). The Eq. (6) then turns into the well-known expression for free oscillations of a harmonic oscillator. Using the dimensionless variables, it can be written in the form:

$$y(\tau, \tilde{\varepsilon} < 1) \cong \mp\sqrt{\tilde{\varepsilon}}\sin(\tau + \varphi). \quad (7)$$

From (5) and (7) it follows that the oscillation period for the Morse oscillator depends on the energy and is given by the expression

$$T^{(Morse)}(\varepsilon) = \frac{2\pi}{\omega_0\sqrt{1 - \tilde{\varepsilon}}}. \quad (8)$$

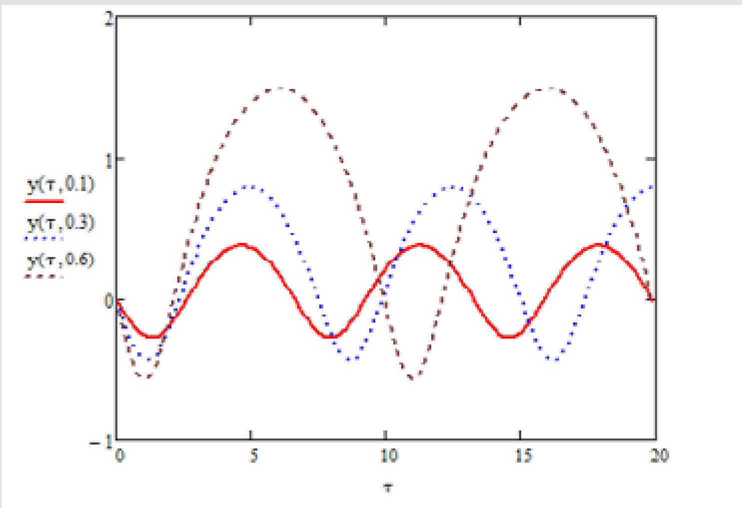

Figure 2: The Morse oscillator's motion for various values of dimensionless energy: $\tilde{\varepsilon} = 0.1$ (solid curve), $\tilde{\varepsilon} = 0.3$ (dotted curve), and $\tilde{\varepsilon} = 0.6$ (dashed curve) and for the negative initial velocity.

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It should be noted that this is the period of anharmonic oscillations. The motion of the Morse oscillator, defined as the dependence of the dimensionless coordinate on the dimensionless time, are shown in (Figure 2) for different values of the dimensionless energy. It is noticeable that when the energy is low, the oscillations are symmetrical in accordance with the Eq. (7) which describes the harmonic oscillator's motion. With energy increasing, the amplitude of oscillations scales up, the motion becomes asymmetric and anharmonic and oscillation period increases. This anharmonicity is explained by the Morse potential energy's asymmetry with respect to the equilibrium coordinate (x = 0 in (Figure 1)) – this asymmetry does ~~is~~ not exist in the harmonic oscillator's potential energy.

Infinite Motion

The Eq. (8) suggests that with the increasing energy, the period also increases, and with $\varepsilon \to D$, $T^{(Morse)} \to \infty$ Thus, upon reaching the boundary of the negative part of the spectrum where $\tilde{\varepsilon} = 1$, the periodic movement of the Morse oscillator becomes aperiodic. The law of motion for the energy laying on this boundary, $\varepsilon = D$, following from (4) in the dimensionless variables is given by the following formula:

$$y(\tau) = \mathrm{h}\left\{\frac{1}{2}\left[1 + \left(\tau \pm \sqrt{2\exp(y_0) - 1}\right)^2\right]\right\}, \quad (9)$$

where $y_0 = y(0)$ is the value of the dimensionless coordinate at the initial moment of time. It is required that $y_0 \geq -\mathrm{h}\ 2$ so that the radicand in the right side of equality (9) is non-negative. The sign plus in (9) relates to positive initial velocity and sign minus to the negative one. When the time tends to infinity, $\tau \to \infty$, the dimensionless coordinate of the Morse oscillator for $\tilde{\varepsilon} = 1$ increases logarithmically: $y \propto \mathrm{h}\ \tau$. In this case, obviously, the dimensionless velocity $\dot{y}_\tau \to 1/\tau$, i.e., it decreases to zero at the infinity, so that the oscillator's energy reduces to zero. For the energies in the positive part of the spectrum where $\tilde{\varepsilon} > 1$, the calculation of the integral in (4) leads to the following law of motion:

$$y(\tau) = \mathrm{h}\left\{\frac{\tilde{\mathrm{v}}^2 + \left[A(\tilde{\mathrm{v}}, y_0)\exp(-\tilde{\mathrm{v}}\tau) - 1\right]^2}{2\tilde{\mathrm{v}}^2 A(\tilde{\mathrm{v}}, y_0)\exp(-\tilde{\mathrm{v}}\tau)}\right\}, \quad (10)$$

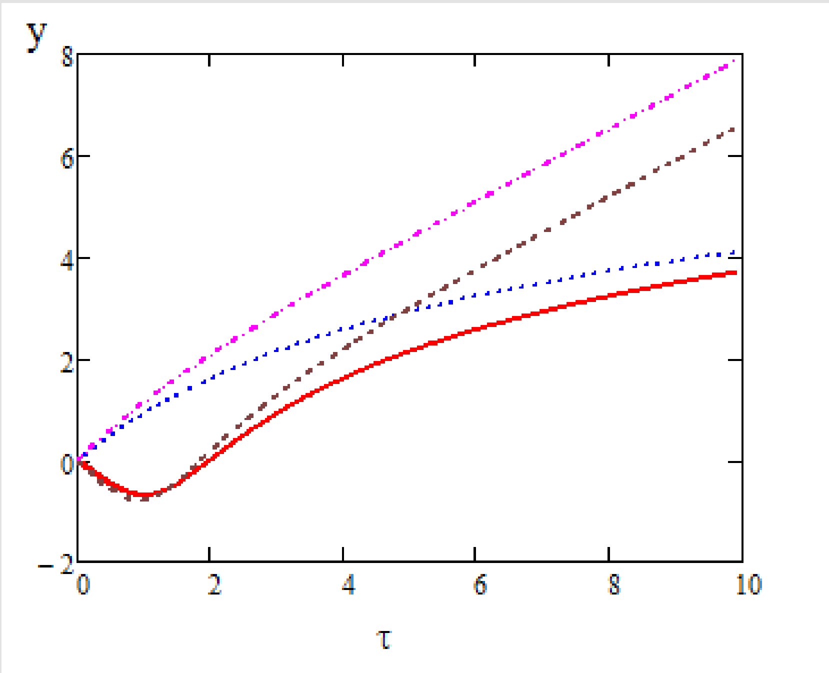

Figure 3: The Morse oscillator's infinite motion for various dimensionless energies and different signs of initial velocity: solid curve - $\tilde{\varepsilon} = 1$, $\dot{y}_0 < 0$, dotted curve - $\tilde{\varepsilon} = 1$, $\dot{y}_0 > 0$; dashed curve - $\tilde{\varepsilon} = 1.5$, $\dot{y}_0 < 0$, dotted-dashed curve - $\tilde{\varepsilon} = 1.5$, $\dot{y}_0 > 0$.

where

$$A(\tilde{v}, y_0) = \tilde{v}^2 \exp(y_0) + 1 \pm \tilde{v} \exp(y_0)\sqrt{\tilde{v}^2 + 2\exp(-y_0) - \exp(-2y_0)} \quad (11)$$

is the constant determined by the initial conditions, and $\tilde{v} = \sqrt{\tilde{\varepsilon} - 1}$ is the dimensionless velocity at infinity. Upper sign in (11) corresponds to negative initial velocity and lower one to the positive initial velocity. From the (10) it follows that when time tends to infinity ($\tau >$ $\tilde{v}^{-1}$), the oscillator's coordinate $y \propto \tilde{v}\tau$. This suggests that when the Morse oscillator's total energy is positive, i.e., when $\tilde{\varepsilon} > 1$, the expansion happens linearly in time. The time dependences of the Morse oscillator's infinite motion are demonstrated in Figure 3. For these graphs, the initial coordinate is assumed to be equal to zero, $y_0 = 0$. The solid and dotted curves for $\tilde{\varepsilon} = 1$ describes the scattering according to the logarithmic law of (9) for a sufficiently long time, $\tau \geq 3$. In this case, $\dot{y} \to 0$ for $\tau \to \infty$, and the energy vanishes at the infinity. The dashed and dotted-dashed curves correspond to the expansion for relative energies greater than one, $\tilde{\varepsilon} > 1$. It can be seen that in these cases the dependence $y(\tau)$ becomes linear when time tends to infinity, i.e., the movement occurs at a constant speed. This follows from (10), as mentioned above. For the negative initial velocity, the function $y(\tau)$ has a minimum. Further analysis shows that with the increase of the initial coordinate, this minimum shifts to the larger values of τ. It should be noted that for the comparison of analytical formulas with numerical solutions for infinite motion one can use the following initial conditions for velocity: $\dot{y}_0(y_0, \tilde{\varepsilon}) = \sqrt{\tilde{\varepsilon} - 1 - \tilde{u}(y_0)}$, for the given energy $\tilde{\varepsilon}$ and coordinate y_0; here $\tilde{u}(y_0) = U(y_0/k)/D$ is normalized potential energy as a function of dimensionless coordinate.

Analogy with the Kepler Problem

The three described modes of Morse oscillator's one-dimensional motion have an extended analogy in the three-dimensional case. Their counterpart is the motion of a particle in a three-dimensional Coulomb attraction field or in a gravitational field. Any movement in such a field can occur in three modes: in an ellipse when the energy is negative, in a parabola when the energy equals to zero, or in a hyperbola when the energy is positive. This motion is known as the Kepler problem. The role of the dimensionless energy $\tilde{\varepsilon} = \varepsilon/D$ in the case of the Kepler problem is determined by the square of the orbit's eccentricity e^2 :

$$e^2 \leftrightarrow \tilde{\varepsilon}. \quad (12)$$

Indeed, in the Kepler case, the total energy $E_K \propto e^2 - 1$, while in the case of the Morse oscillator, $E_M \propto \tilde{\varepsilon} - 1$. As it is known [5], when $e^2 < 1$, the movement occurs on an ellipse, when $e^2 = 1$ – on a parabola, and when $e^2 > 1$ – on a hyperbola. It is obvious that in this model, $e > 0$. These movement types are in accordance with the abovementioned Morse oscillator's free motion modes. For the period of motion along an ellipse, we have $T^{(Kepler)}(e) \propto (1 - e^2)^{-3/2}$, and for the period of Morse oscillations, we have $T^{(Morse)}(\tilde{\varepsilon}) \propto (1 - \tilde{\varepsilon})^{-1/2}$. When the eccentricity or the dimensionless energy approaches one, the period of motion tends to infinity for both models, although according to different laws. We would like to also note that if the eccentricity is zero in the Kepler problem, $e = 0$, the motion happens along a circle. However, if $\tilde{\varepsilon} = 0$, the coordinate of the Morse oscillator turns to zero in accordance with the (5). The circle in the Kepler problem converts into a single point for the Morse oscillator. When moving along a hyperbola when $E_K > 0$, we have the following asymptotic dependence for the radius vector in the Kepler problem when time tends to infinity: $r(t \to \infty) \to \sqrt{2E_K/m}\, t$ (here m is reduced mass of Kepler problem). The movement hence occurs at a constant speed, same as in the expansion case for the Morse oscillator when $\tilde{\varepsilon} > 1$, in accordance with (10). Thus, the free motion modes of the Morse oscillator for both oscillations and expansion can be considered as a one-dimensional analogue of the two-dimensional motion in the Kepler problem. These motions have the same qualitative dependencies, though are described by different formulas. It is worth noting that for both oscillations and expansion, relatively simple explicit expressions were obtained to describe the motion. This explicitness and simplicity are not always possible for other types of potential [4,5].

Conclusion

The analytical formulas describing the Morse oscillator's free motion in dimensionless variables have been derived and analyzed. In addition to the previous results [2,3] we took into account different signs of the initial oscillator's velocity. Further to that, our formulas explicitly depend on the initial conditions, which makes it easy to compare them with the results of a numerical solution to this problem. The study involved three motion modes: oscillatory, infinite with zero energy, and infinite with positive energy. The analysis involved motion characteristics of each of these cases. For the oscillatory mode, the relation between the period of a Morse oscillator and its energy has been established. The analogy between the Morse oscillator's free motion and the motion of a particle in a gravitational potential, i.e., the Kepler problem, has been demonstrated.

Competing Interests

The authors declare that they have no competing interests.

Authors' Contributions

The authors wrote, read and approved the final manuscript.

References

1. LD Landau, E M Lifshitz (1965) Quantum Mechanics (Pergamon Press Oxford).
2. WC DeMarcus (1978) Classical motion of Morse oscillator. Am J Phys 46(7): 733-734.
3. FL Moraes Barboza, AJ Costa, NF Ribeiro, ED Filho (2007) Analytical solution of the Morse potential in classical mechanics. Rev Bras Ensino Fís 29(4): 543-547.
4. VA Astapenko (2011) Interaction of the Radiation with Atoms and Nanoparticles (Intellect. Dolgoprudny) 112(2): 193-198.
5. LD Landau, EM Lifshitz (1961) Mechanics (Pergamon Press Oxford).

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