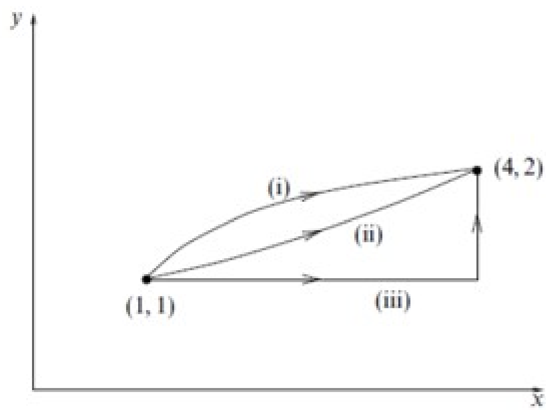
Tutorial 8

1 Work as path integral

Calculate the work by the force $\boldsymbol{F} = (x+y)\,\hat{\boldsymbol{x}} + (y-x)\,\hat{\boldsymbol{y}}$ along the following trajectories:

1. The parabola $y^2 = x$ between $(1,1)$ to $(4,2)$.
2. The curve $x = 2u^2 + u + 1$, $y = 1 + u^2$ between $(1,1)$ to $(4,2)$.
3. The line $y = 1$ between $(1,1)$ to $(4,1)$ and then the line $x = 4$ between $(4,1)$ to $(4,2)$.



Solution:

Our trajectories are in the $x-y$ plane so $\boldsymbol{dl} = dx\hat{\boldsymbol{x}} + dy\hat{\boldsymbol{y}}$ and we want to find a single variable to help us express dx, dy, and $\boldsymbol{F}$.

1. We can choose our variable to be y and if we set the limits to be $y : 1 \to 2$ so $(x,y) = \left(y^2, y\right) : (1,1) \to (4,2) \Rightarrow$

$$W = \int_{(1,1)}^{(4,2)} \boldsymbol{F} \cdot \boldsymbol{dl} = \int_1^2 \left(y + y^2, y - y^2\right) \cdot (2ydy, dy) =$$

$$= \int_1^2 2\left(y^2 + y^3\right) dy + \int_1^2 \left(y - y^2\right) dy = \int_1^2 \left(2y^3 + y^2 + y\right) dy =$$

$$= \left[2\frac{y^4}{4} + \frac{y^3}{3} + \frac{y^2}{2}\right]_1^2 = 11\frac{1}{3}\text{ J.}$$

2. We can choose our variable to be u and the trajectory element vector becomes

$$\begin{aligned} x &= 2u^2 + u + 1 \\ y &= 1 + u^2 \end{aligned} \quad \Rightarrow \quad \begin{aligned} dx &= (4u+1)\,du \\ dy &= 2udu \end{aligned}$$

One can also find the limits on u by setting $u=0$ where $(x,y)=(1,1)$ and setting $u=1$ where $(x,y)=(4,2)$. Then we get $u:0\to 1$.

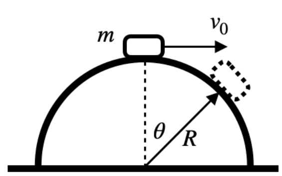
$$W=\int_{(1,1)}^{(4,2)}\boldsymbol{F}\cdot\boldsymbol{dl}=\int_0^1\left(3u^2+u+2,-u-u^2\right)\cdot(4u+1,2u)\,du=$$
$$=\int_0^1\left[\left(3u^2+u+2\right)(4u+1)-\left(u+u^2\right)2u\right]du=\int_0^1\left[10u^3+5u^2+9u+2\right]du=$$
$$=10\frac{2}{3}\text{ J.}$$

3. Here we separate our trajectory into 2 parts. In the first one our variable will be x while $y=const\Rightarrow dy=0$, and in the second part y is the variable and $x=const\Rightarrow dx=0$.

$$W=\int_{(1,1)}^{(4,2)}\boldsymbol{F}\cdot\boldsymbol{dl}=\int_1^4\boldsymbol{F}\cdot\boldsymbol{dx}+\int_1^2\boldsymbol{F}\cdot\boldsymbol{dy}=$$
$$=\int_1^4 1+x\,dx+\int_1^2 y-4\,dy=\left[x+\frac{x^2}{2}\right]_1^4+\left[\frac{y^2}{2}-4y\right]_1^2=10.5-2.5$$
$$=8\,\text{J.}$$

2 Sliding on Dome

A body with mass m is sliding on a spherical dome with radius R, under the influence of gravity. It is known that the body begins its motion with initial velocity v_0, as shown in the figure.



1. What is the work done by the gravitational force as a function of the angle θ to the body?
2. What is the kinetic energy of the body at angle θ?
3. What are the radial and tangent accelerations?
4. At what angle will the body part from the dome?

Solution:

1. Setting the zero potential energy to be at at the base of the dome, we can write the potential energy as

$$W_g=\int m\boldsymbol{g}\cdot d\boldsymbol{\ell}=\int_0^{\theta}mgR\sin\left(\theta'\right)\,d\theta'=mgR\left(1-\cos\theta\right).$$

2. Because the only force, with a component in the direction of the motion of the body is gravity, we find

$$\Delta E_k = \sum_i W_i = mgR\left(1-\cos\theta\right)$$

thus

$$E_k\left(\theta\right) = \frac{1}{2}mv_0^2 + mgR\left(1-\cos\theta\right).$$

3. Since the only force tangent to the direction of motion is mg, we find, using $\boldsymbol{F} = m\boldsymbol{a}$, that

$$a_T = g\sin\theta.$$

Whereas the radial acceleration is $a_r = -R\dot{\theta}^2$ (since $\dot{r} = \ddot{r} = 0$), thus

$$a_r = -\frac{v^2}{R} = -\frac{2}{mR}E_k\left(\theta\right) = -\frac{2}{mR}\left[\frac{1}{2}mv_0^2 + mgR\left(1-\cos\theta\right)\right] = -\left[\frac{v_0^2}{R} + 2g\left(1-\cos\theta\right)\right].$$

4. The body parts from the dome when the normal force vanishes, i.e. $N = 0$, which yields

$$-mg\cos\theta = ma_r \quad \rightarrow \quad g\cos\theta = \frac{v_0^2}{R} + 2g\left(1-\cos\theta\right).$$

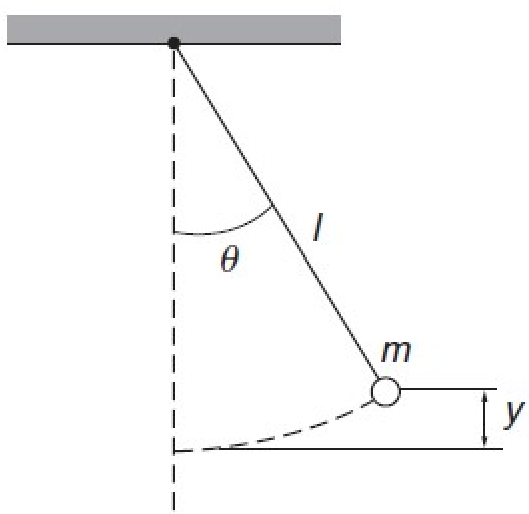
Solving for θ, we find

$$\cos\theta = \frac{1}{3}\left(\frac{v_0^2}{gR} + 2\right).$$

Checking our result we see that when $\frac{v_0^2}{gR} > 1$ there is no solution for θ. This because the body does not slide on the dome right from the start, instead it shoots off into the air immediately.

3 Pendulum Motion

A simple pendulum - a point mass M hanging from a massless string of length l - moves in a circular arc in a vertical plane.
Find $\theta(t)$ using energy considerations given that the maximal angle of the pendulum swing is θ_0 and that at $t = 0$, $\theta = 0$.
*You can assume $\theta_0 \ll 1$.



Solution:

The kinetic energy for θ_0

$$K_{\theta_0} = 0$$

because that's where the motion changes direction.
At some different θ

$$K_\theta = \frac{1}{2} M \left(l\dot{\theta} \right)^2$$

The forces on M are tension $T\left(-\sin\theta, \cos\theta\right)$ for some θ of the motion, and the gravitational force $Mg\left(0, -1\right)$

The location of the mass is given by $\overrightarrow{r} = l\left(\sin\theta, 1 - \cos\theta\right)$ then the element of the trajectory of the mass is given by $l\left(\cos\theta, \sin\theta\right) d\theta$

Using the work-energy theorem

$$\Delta K = \frac{1}{2} M \left(l\dot{\theta} \right)^2 = \int_{\theta_0}^{\theta} \left[T\left(-\sin\theta, \cos\theta\right) + \left(0, -Mg\right) \right] \cdot \left(\cos\theta, \sin\theta\right) l d\theta =$$

$$= \int_{\theta_0}^{\theta} -Mg \sin\theta \, l d\theta = Mgl\left(\cos\theta - \cos\theta_0\right)$$

For small angles $\cos\theta \approx 1 - \frac{1}{2}\theta^2$
And we get the differential equation

$$\frac{1}{2} M \left(l\dot{\theta} \right)^2 = \frac{1}{2} Mgl \left(\theta_0^2 - \theta^2 \right)$$

$$\dot{\theta} = \sqrt{\frac{g}{l}} \sqrt{\theta_0^2 - \theta^2}$$

$$\frac{\frac{d\theta}{\theta_0}}{\sqrt{1 - \left(\frac{\theta}{\theta_0}\right)^2}} = \frac{d\theta}{\sqrt{\theta_0^2 - \theta^2}} = \sqrt{\frac{g}{l}} dt$$

The integral on the left has the form $\int dx / \sqrt{1 - x^2} = \arcsin x$, where $x = \frac{\theta}{\theta_0}$

$$\arcsin \frac{\theta}{\theta_0} - 0 = \sqrt{\frac{g}{l}} \left(t - 0\right)$$

$$\theta(t) = \theta_0 \sin\left(\sqrt{\frac{g}{l}} t \right)$$

Notice that $\omega = \sqrt{\frac{g}{l}}$ is the frequency of the pendulum.

4 Conservative Force

1. Given the following force

$$\boldsymbol{F} = f_0 \left(y\hat{\boldsymbol{x}} - x\hat{\boldsymbol{y}} \right),$$

   (a) Is the force conservative?
   (b) A particle positioned at $(R, 0)$ is moving along a circle with radius R counterclockwise, up to the point $(0, R)$. What is the work done by the force?
   (c) Repeat (b) when the particle moves backwards.

2. Given the following force

$$\boldsymbol{F} = -k\frac{x\hat{\boldsymbol{x}} + y\hat{\boldsymbol{y}} + z\hat{\boldsymbol{z}}}{(x^2 + y^2 + z^2)^{3/2}},$$

   (a) Show that the force is conservative (you may ignore the singularity at $(0, 0, 0)$).

   (b) Find the potential function U for the force.

   (c) A body moves from position $(0, 0, L)$ to the position (L, L, L) in a straight line. Calculate the work done, using path integral.

   (d) Repeat (c), this time using the potential function.

Solution:

1. For the force $\boldsymbol{F} = f_0\,(y\hat{\boldsymbol{x}} - x\hat{\boldsymbol{y}})$:

   (a) In order to find if $\boldsymbol{F}$ is conservative we evaluate its rotor,

$$\boldsymbol{\nabla} \times \boldsymbol{F} = (\partial_x F_y - \partial_y F_x)\,\hat{\boldsymbol{z}} = (-f_0 - f_0)\,\hat{\boldsymbol{z}} = -2f_0\hat{\boldsymbol{z}} \neq 0,$$

   thus $\boldsymbol{F}$ is not a conservative force.

   (b) The work done by $\boldsymbol{F}$ is

$$W = \int \boldsymbol{F} \cdot d\boldsymbol{r}.$$

   Let us evaluate the integral in polar coordinates:

$$\begin{aligned} x &= R\cos\theta \\ y &= R\sin\theta \\ \hat{\boldsymbol{x}} &= \cos\theta\hat{\boldsymbol{r}} - \sin\theta\hat{\boldsymbol{\theta}} \\ \hat{\boldsymbol{y}} &= \sin\theta\hat{\boldsymbol{r}} + \cos\theta\hat{\boldsymbol{\theta}}, \end{aligned}$$

   which reads

$$\begin{aligned} \boldsymbol{F} &= f_0\left[R\sin\theta\left(\cancel{\cos\theta\hat{\boldsymbol{r}}} - \sin\theta\hat{\boldsymbol{\theta}}\right) - R\cos\theta\left(\cancel{\sin\theta\hat{\boldsymbol{r}}} + \cos\theta\hat{\boldsymbol{\theta}}\right)\right] \\ &= -f_0 R\left[-\sin^2\theta\hat{\boldsymbol{\theta}} - \cos^2\theta\hat{\boldsymbol{\theta}}\right] \\ &= -f_0 R\hat{\boldsymbol{\theta}}. \end{aligned}$$

   We also need to write $d\boldsymbol{r}$ properly as

$$\begin{aligned} d\boldsymbol{r} &= dx\hat{\boldsymbol{x}} + dy\hat{\boldsymbol{y}} \\ &= (dr\cos\theta - rd\theta\sin\theta)\,\hat{\boldsymbol{x}} + (dr\sin\theta + rd\theta\cos\theta)\,\hat{\boldsymbol{y}} \\ &= dr\,(\cos\theta\hat{\boldsymbol{x}} + \sin\theta\hat{\boldsymbol{y}}) + rd\theta\,(\cos\theta\hat{\boldsymbol{y}} - \sin\theta\hat{\boldsymbol{x}}) \\ &= dr\hat{\boldsymbol{r}} + rd\theta\hat{\boldsymbol{\theta}}, \end{aligned}$$

   in our case the motion is only in the angular direction, therefore $dr = 0$, i.e. $d\boldsymbol{r} = Rd\theta\,\hat{\boldsymbol{\theta}}$.

Therefore,

$$\begin{aligned}
W &= \int \boldsymbol{F} \cdot d\boldsymbol{r} \\
&= -\int_0^{\pi/2} \left(f_0 R \hat{\boldsymbol{\theta}}\right) \cdot \left(R d\theta\, \hat{\boldsymbol{\theta}}\right) \\
&= -\int_0^{\pi} f_0 R^2 d\theta \\
&= -\frac{\pi}{2} f_0 R^2.
\end{aligned}$$

(c) Since the only thing that changes is the direction of the motion (the force remain the same in each point on the path) then the work is simply

$$W = +\frac{\pi}{2} f_0 R^2.$$

2. For the force $\boldsymbol{F} = -k\frac{x\hat{\boldsymbol{x}}+y\hat{\boldsymbol{y}}+z\hat{\boldsymbol{z}}}{(x^2+y^2+z^2)^{3/2}}$,

(a) In order to find if $\boldsymbol{F}$ is conservative we evaluate its rotor,

$$\begin{aligned}
\boldsymbol{\nabla} \times \boldsymbol{F} &= \left(\partial_y F_z - \partial_z F_y\right)\hat{\boldsymbol{x}} + \left(\partial_z F_x - \partial_x F_z\right)\hat{\boldsymbol{y}} + \left(\partial_x F_y - \partial_y F_x\right)\hat{\boldsymbol{z}} \\
&= \left(-k\frac{z\,(-3/2)\,2y}{(x^2+y^2+z^2)^{5/2}} + k\frac{y\,(-3/2)\,2z}{(x^2+y^2+z^2)^{5/2}}\right)\hat{\boldsymbol{x}} + (\dots)\,\hat{\boldsymbol{y}} + (\dots)\,\hat{\boldsymbol{z}} \\
&= 0.
\end{aligned}$$

(b) We need to find U such that $\boldsymbol{F} = -\boldsymbol{\nabla} U$. Looking at the x direction

$$F_x = -k\frac{x}{(x^2+y^2+z^2)^{3/2}} = -\partial_x U,$$

integration yields

$$\begin{aligned}
U(x,y,z) &= \int k\frac{x}{(x^2+y^2+z^2)^{3/2}} dx \\
&\begin{cases} s \equiv x^2+y^2+z^2 \\ ds = 2x dx \end{cases} \\
&= \frac{k}{2}\int \frac{1}{s^{3/2}} ds \\
&= -k\frac{1}{s^{1/2}} + C_x(y,z) \\
U(x,y,z) &= -k\frac{1}{(x^2+y^2+z^2)^{1/2}} + C_x(y,z).
\end{aligned}$$

Following the same routine for y and z yields

$$U(x,y,z) = -k\frac{1}{(x^2+y^2+z^2)^{1/2}} + C_y(x,z) \quad \text{and} \quad U(x,y,z) = -k\frac{1}{(x^2+y^2+z^2)^{1/2}} + C_z(x,y),$$

which means $C_x(y,z) = C_y(x,z) = C_z(x,y)$. The only possible solution is a constant C, thus the potential is

$$U(x,y,z) = -k\frac{1}{(x^2+y^2+z^2)^{1/2}} + C,$$

and since a constant shift in the potential does not affect physical results, which depend only on potential differences, we may write it simply as

$$U(x,y,z) = -k\frac{1}{(x^2+y^2+z^2)^{1/2}}.$$

Another way:
As before, we first use the equation in the x direction

$$F_x(x,y,z) = -\frac{\partial}{\partial x}U(x,y,z) \quad \rightarrow \quad U(x,y,z) = -\int F_x dx = -\frac{k}{(x^2+y^2+z^2)^{1/2}} + h(y,z),$$

where $h(y,z)$ is any general function of y and z, so that be calculating dU/dx we always get back F_x since $dh(y,z)/dx = 0$.
Next we turn to the equation for the y direction

$$F_y(x,y,z) = -\frac{\partial}{\partial y}U(x,y,z) = -\frac{\partial}{\partial y}\left[-\frac{k}{(x^2+y^2+z^2)^{1/2}} + h(y,z)\right] = -k\frac{y}{(x^2+y^2+z^2)^{3/2}} - \frac{\partial}{\partial y}h(y,z),$$

plugging in the expression for $F_y$we find

$$-k\frac{y}{(x^2+y^2+z^2)^{3/2}} - \frac{\partial}{\partial y}h(y,z) = -k\frac{y}{(x^2+y^2+z^2)^{3/2}} \quad \rightarrow \quad \frac{\partial}{\partial y}h(y,z) = 0,$$

thus

$$h(y,z) = g(z),$$

where $g(z)$ is a function of z alone, since $h(y,z)$ is a function of y and z alone and $\partial h/\partial y = 0$.
Finally we turn to the equation in the z direction

$$F_z(x,y,z) = -\frac{\partial}{\partial z}U(x,y,z) = -\frac{\partial}{\partial z}\left[-\frac{k}{(x^2+y^2+z^2)^{1/2}} + g(z)\right] = -k\frac{z}{(x^2+y^2+z^2)^{3/2}} - \frac{\partial}{\partial z}g(z),$$

plugging in the expression for F_z we find

$$-k\frac{z}{(x^2+y^2+z^2)^{3/2}} - \frac{\partial}{\partial z}g(z) = -k\frac{z}{(x^2+y^2+z^2)^{3/2}} \quad \rightarrow \quad \frac{\partial}{\partial z}g(z) = 0,$$

thus

$$g(z) = C,$$

where C is a constant. Therefore, after using all three equations we find

$$U(x,y,z) = -\frac{k}{(x^2+y^2+z^2)^{1/2}} + C,$$

for which we can choose $C = 0$, since a constant does not affect physical quantities which depend on energy differences alone.

(c) Although the required path is a straight line, we've found that the force $\boldsymbol{F}$ is conservative, thus we may evaluate the work in any desired path - the simplest is by moving in two segments

$(0,0,L) \to (0,L,L) \to (L,L,L)$:

$$
\begin{aligned}
W &= \int \boldsymbol{F} \cdot d\boldsymbol{r} \\
&= \int_0^L \boldsymbol{F} \cdot d\boldsymbol{y} + \int_0^L \boldsymbol{F} \cdot d\boldsymbol{x} \\
&= \int_0^L \left(-k \frac{0\cancel{\hat{\boldsymbol{x}}} + y\hat{\boldsymbol{y}} + L\cancel{\hat{\boldsymbol{z}}}}{(0^2 + y^2 + L^2)^{3/2}} \right) \cdot d\boldsymbol{y} + \int_0^L \left(-k \frac{x\hat{\boldsymbol{x}} + L\cancel{\hat{\boldsymbol{y}}} + L\cancel{\hat{\boldsymbol{z}}}}{(x^2 + L^2 + L^2)^{3/2}} \right) \cdot d\boldsymbol{x} \\
&= -\int_0^L k \frac{y}{(y^2 + L^2)^{3/2}} dy - k \int_0^L \frac{x}{(x^2 + 2L^2)^{3/2}} dx \\
&= -k \left[\frac{-1}{(y^2 + L^2)^{1/2}} \Big|_0^L + \frac{-1}{(x^2 + 2L^2)^{1/2}} \Big|_0^L \right] \\
&= -k \left[\cancel{\frac{-1}{\sqrt{2L^2}}} + \frac{1}{L} + \frac{-1}{\sqrt{3L^2}} + \cancel{\frac{1}{\sqrt{2L^2}}} \right] \\
&= \frac{k}{L} \left(\frac{1}{\sqrt{3}} - 1 \right).
\end{aligned}
$$

(d) Using the potential, all we need to do is evaluate the potential difference

$$
W = U(0,0,L) - U(L,L,L) = -k \frac{1}{(L^2)^{1/2}} + k \frac{1}{(3L^2)^{1/2}} = \frac{k}{L} \left(\frac{1}{\sqrt{3}} - 1 \right),
$$

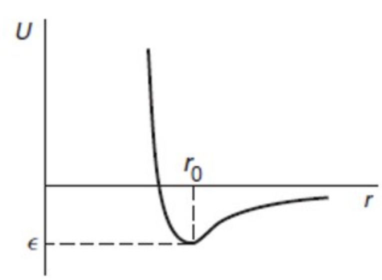
which is the same as (c).

5 Lennard-Jones Potential

A commonly used potential energy function to describe the interaction between two atoms is the Lennard-Jones potential given by

$$
U = \epsilon \left[\left(\frac{r_0}{r} \right)^{12} - 2 \left(\frac{r_0}{r} \right)^6 \right]
$$

1. Find the position of the potential minimum and its value.
2. Near the minimum the atoms execute simple harmonic motion. Find the frequency of oscillation.
3. Find a range of values for the system energy for which atoms will move in bounded trajectories.
4. For a given energy E that is in the range you found above, find the distances r between the two atoms that are turning points.



Solution:

1. Differentiating U
$$\frac{dU}{dr} = \epsilon\left[-12\left(\frac{r_0^{12}}{r^{13}}\right) + 12\left(\frac{r_0^6}{r^7}\right)\right]$$
$\frac{dU}{dr} = 0$ for $r = r_0$.
Substituting $r = r_0$ in U
$$U(r_0) = -\epsilon.$$

2. In order to find the frequency of oscillations we will use the spring model near the minimum point r_0, where
$$U(r) = \underbrace{U(r_0)}_{\text{constant}} + \cancel{U'(r = r_0)}(r - r_0) + \frac{1}{2}U''(r = r_0)(r - r_0)^2 \cdots \approx \frac{1}{2}k\Delta r^2 \quad \rightarrow \quad k = U''(r = r_0)$$
and since we know that, for the spring model,
$$\omega^2 = \frac{k}{\mu},$$
where μ is the mass of oscillating object, thus
$$\omega = \sqrt{\left(\frac{d^2U}{dr^2}\right)_{r=r_0}\frac{1}{\mu}}.$$
Since the potential depends on the distance between the two atoms it is easier to choose the frame of reference of one of these atoms, so that the distance between the atoms $\boldsymbol{r} = |\boldsymbol{r}_1 - \boldsymbol{r}_2|$ will be our new coordinate and we can deal only with the motion of one atom instead of both. Doing so we must take into account that the relative acceleration $\boldsymbol{a}_{\text{rel}}$ as well. Let us note that the second and third Newtons laws read
$$\boldsymbol{F}_{12} = m_1\ddot{\boldsymbol{r}}_1 \quad \boldsymbol{F}_{21} = m_1\ddot{\boldsymbol{r}}_2 \quad \text{and} \quad \boldsymbol{F}_{12} = -\boldsymbol{F}_{21},$$
hence
$$\ddot{\boldsymbol{r}}_2 = -\frac{m_1}{m_2}\ddot{\boldsymbol{r}}_1.$$
Therefore, the relative acceleration is
$$\boldsymbol{a}_{\text{rel}} = \ddot{\boldsymbol{r}} = \ddot{\boldsymbol{r}}_1 - \ddot{\boldsymbol{r}}_2 = \left(1 + \frac{m_1}{m_2}\right)\ddot{\boldsymbol{r}}_1 = \frac{m_1 + m_2}{m_1 m_2}\underbrace{m_1\ddot{\boldsymbol{r}}_1}_{\boldsymbol{F}_{12}} = \frac{m_1 + m_2}{m_1 m_2}\boldsymbol{F}_{12}.$$
Thus, the motion of atom m_1 is described by the equation
$$\boldsymbol{F}_{12} = \frac{m_1 m_2}{m_1 + m_2}\boldsymbol{a}_{\text{rel}} \quad \Longleftrightarrow \quad \boldsymbol{F} = \mu\boldsymbol{a},$$
where $\mu = \frac{m_a}{2}$ and $m_a = m_1 = m_2$ is the mass of each atom.
Getting back to the expression for ω,
$$\left(\frac{d^2U}{dr^2}\right)_{r=r_0} = \epsilon\left[156\left(\frac{r_0^{12}}{r^{14}}\right) - 84\left(\frac{r_0^6}{r^8}\right)\right]_{r=r_0} = \epsilon\,[156 - 84] = 72\epsilon$$
And we get
$$\omega = \sqrt{\frac{144\epsilon}{m_a}}.$$

3. For $r \rightarrow \infty$ $U \rightarrow 0$. Therefore, for energies in the range $-\epsilon < E < 0$ the motion of the atoms will be bounded.

4. We need to find the distances between the two atoms where $U(r) = E\,(< 0)$. $E = -|E|$ and $|E| < \epsilon$

$$-|E| = \epsilon\left[\left(\frac{r_0}{r}\right)^{12} - 2\left(\frac{r_0}{r}\right)^{6}\right]$$

Multiplying by r^{12}

$$-|E|\,r^{12} + 2\epsilon r_0^6 r^6 - \epsilon r_0^{12} = 0$$

$$r^{12} - 2\frac{\epsilon}{|E|}r_0^6 r^6 + \frac{\epsilon}{|E|}r_0^{12} = 0$$

This is a quadratic equation for r^6.

$$r^6 = \left[\frac{\epsilon}{|E|}r_0^6 \pm \sqrt{\left(\frac{\epsilon}{|E|}\right)^2 r_0^{12} - \frac{\epsilon}{|E|}r_0^{12}}\right] = \frac{\epsilon}{E}r_0^6\left[1 \pm \sqrt{1 - \frac{|E|}{\epsilon}}\right].$$