PHYS 3803: Quantum Mechanics I, Spring 2021 Week 1: January 25 (M)–January 29 (F)

Lecture 1, January 26, 2021 (Tuesday)

- Handouts: Syllabus (Check your OU Email)
- Midterm Exam: March 12 (Friday), 1:30 p.m.–3:30 p.m.
- Final Exam: May 11 (Tuesday), 1:30 p.m.–3:30 p.m.
- Reading: Study Lagrangian and Hamiltonian Dynamics with your favorite Classical Mechanics textbook.
- Assignment: Problem Set 1 due February 03 (Wednesday). Make a pdf file and send it to our grader: jmderkacy@ou.edu

Topics for Today: Review of Classical Mechanics

- A The Hamiltonian and Quantum Mechanics
- 1.1 The Lagrangian, the Action, and Hamilton's Principle
- 1.2 Functional Derivatives
- 1.3 Back to Hamilton's Principle
- 1.4 More Degrees of Freedom
- 1.5 The Euler-Lagrange Equation
- 1.6 The Lagrangian and the Sum Over Paths

Topics for Quantum Mechanics I

- 1 Review of Classical Mechanics [Taylor 7, 13]
- 2 Mathematical Tools [Griffiths 3]
- 3 One-dimensional Schrödinger Equation [Griffiths 1 and 2]
- 4 Harmonic Oscillator [Griffiths 2.3]
- 5 Angular Momentum [Griffiths 4.1 and 4.3]
- 6 Hydrogen Atom [Griffiths 4.2]
- 7 BONUS: Path Integral
- 8 Symmetries and Conservation Laws [Griffiths 6]

Canonical Momentum and the Hamiltonian

Recall that $T(q, \dot{q}, t)$ = the kinetic energy, $U(q, \dot{q}, t)$ = the potential energy, and the Lagrangian is defined as

$$L(q, \dot{q}, t) \equiv T(q, \dot{q}, t) - U(q, \dot{q}, t) \,.$$

With the conjugate momentum or the canonical momentum $p_i \equiv \partial L/\partial \dot{q}_i$, the Legendre transformation takes $L(q_i, \dot{q}_i, t)$ to $H(q_i, \partial L/\partial \dot{q}_i, t) = H(q_i, p_i, t)$.

The Hamiltonian is defined as

$$H(q, p, t) \equiv \sum_{i} \dot{q}_{i} \left(\frac{\partial L}{\partial \dot{q}_{i}}\right) - L(q, \dot{q}, t) = \sum_{i} \dot{q}_{i} p_{i} - L(q, \dot{q}, t) \,.$$

Physical momentum $(\vec{p} = m\vec{v})$ and canonical momentum $(P_i \equiv \partial L/\partial \dot{q}_i)$ are different if the potential energy depends on \dot{q}_i .

Formalism in Quantum Mechanics

A. The Hamiltonian and Quantum Mechanics

The most common formalism in Quantum Mechanics is **Canonical Quantization** or **Operator Formalism**.

A quantum system is described with a state vector $|\psi(t)\rangle$ that becomes a wave function $\psi(\vec{x}, t)$ in coordinate basis, and the equation of motion is the Schrödinger equation

$$\begin{split} H|\psi(t)\rangle &= E|\psi(t)\rangle, \quad (\text{Hilbert space}), \\ H\psi(\vec{x},t) &= E\psi(\vec{x},t), \quad (\text{Coordinate space}), \\ H &= \frac{P^2}{2m} + U, \quad P \equiv -i\hbar\nabla, \quad \text{and} \quad E \equiv i\hbar\frac{\partial}{\partial t}, \end{split}$$

where H = Hamiltonian, and $\psi(\vec{x}, t) =$ the wave function in the coordinate basis. In addition, the quantum operators of every coordinate and its conjugate momentum satisfy the canonical commutation relation

$$[X,P] \equiv XP - PX = i\hbar,$$

and the uncertainty principle

$$\Delta X \Delta P \ge \frac{\hbar}{2},$$

where $\hbar = h/(2\pi)$, and $h \equiv$ Planck's constant.

Let us consider classical observables as continuous functions of generalized coordinates and conjugate momenta: $\omega(q, p)$, $\omega_1(q, p)$ and $\omega_2(q, p)$ where q and p are vectors with components q_k and p_k , $k = 1, \dots, N$. The Poisson brackets are defined as

$$\{\omega_1, \omega_2\} \equiv \sum_{k=1}^{N} \left(\frac{\partial \omega_1}{\partial q_k} \frac{\partial \omega_2}{\partial p_k} - \frac{\partial \omega_1}{\partial p_k} \frac{\partial \omega_2}{\partial q_k} \right).$$

Quantum correspondence principle is the relation between quantum commutators and Poisson brackets:

 $[\Omega_1, \Omega_2] = i\hbar\{\omega_1, \omega_2\}.$

That means, the commutation relation of two quantum operators is $i\hbar$ times the value of the classical Poisson bracket.

It is clear at this point that the Planck's constant \hbar measures the non-classical nature of systems. More commonly we say that we recover classical mechanics in the limit $\hbar \to 0$.

Exercise: Let us consider X, P as quantum operators, show that

 $[X,P] = i\hbar\{x,p\} = i\hbar.$

1 Review of Classical Mechanics

1.1 Lagrangian, Action, and Hamilton's Principle

Let us consider one dimensional motion of a particle with coordinate x(t) and velocity $v(t) = \dot{x}(t)$ in a potential U(x). The kinetic energy is

$$T(x,\dot{x}) = \frac{1}{2}m\dot{x}^2$$

and the potential energy is $U(x, \dot{x})$.

In general, the Lagrangian is defined as

$$L(x, \dot{x}) \equiv T(x, \dot{x}) - U(x, \dot{x}).$$

For a system with a conservative force, the Lagrangian becomes

$$L(x, \dot{x}) \equiv T(\dot{x}) - V(x) \,.$$

It is a scalar, i.e., it is invariant under Lorentz transformation.

The action (S) of a particle moving along along a trajectory [x(t)] is

$$S[x] \equiv \int_{t_a}^{t_b} L(x, \dot{x}) \, dt \, .$$

Hamilton's principle is the statement that the action (S) for a particle moving from x_a at t_a to x_b at t_b

$$S[x] \equiv \int_{t_a}^{t_b} [T(x(t), \dot{x}(t)) - U(x(t), \dot{x}(t))] dt$$

along a path x(t) is stationary (minimum or maximum) for the actual classical trajectory $x(t) = x_0(t)$ that follows Newton's law of motion. Note that

(a). $L \equiv T - U \equiv$ the Lagrangian is a function of two variables: x and \dot{x} .

(b). $S[x] \equiv$ the action is a function whose argument is itself a function. A function of function is sometimes called a functional.

(c). The action S[x] is stationary for the classical trajectory $x_0(t)$.

Taylor Expansion: Taylor expansion is the most useful mathematical formula for physicists.

A function can be approximated by polynomials in the neighborhood of a point (x₀) in terms of its value and derivatives using Taylor expansion about x₀ with f(x) = f(x₀ + Δx):

$$f(x_0 + \Delta x) = f(x_0) + \Delta x \frac{df}{dx}(x_0) + \mathcal{O}[(\Delta x)^2] = \sum_{n=0}^{\infty} \frac{(\Delta x)^n}{n!} \frac{d^n f}{dx^n}(x_0).$$

• For a function of two variables the Taylor expansion becomes

$$f(x,y) = f(x_0 + \Delta x, y_0 + \Delta y)$$

= $f(x_0, y_0) + \Delta x \frac{\partial f}{\partial x}(x_0, y_0) + \Delta y \frac{\partial f}{\partial y}(x_0, y_0)$
+ $\frac{1}{2} \left[(\Delta x)^2 \frac{\partial^2 f}{\partial x^2} + (\Delta y)^2 \frac{\partial^2 f}{\partial y^2} + 2\Delta x \Delta y \frac{\partial^2 f}{\partial x \partial y} \right] + \mathcal{O}(\Delta^3).$

1.2 Functional Derivatives

For the functional

$$W[x] = \int_{t_a}^{t_b} F(x(t), \dot{x}(t)) dt,$$

the functional derivative of W[x] with respect to x(t) is defined as $\delta W[x]/\delta x(t) \equiv$ the coefficient of the linear term in $\delta x(t)$ in $W[x + \delta x]$. The functional derive becomes

$$\frac{\delta W[x]}{\delta x(t)} \equiv \lim_{\delta x \to 0} \frac{W[x + \delta x] - W[x]}{\delta x(t)} = \frac{\partial F}{\partial x} - \frac{d}{dt} \left(\frac{\partial F}{\partial \dot{x}}\right) \,.$$

We can write

$$\frac{\delta W[x]}{\delta x(t)}|_{x=x_0} = \frac{\delta W}{\delta x(t)}[x_0]$$

for the path with $x_0(t)$.

For

$$W[x] = \int_{t_a}^{t_b} [x(t) - t]^2 dt$$
,

we have

$$\frac{\delta W[x_0]}{\delta x(t)} = 2[x_0(t) - t],$$

where we should have applied a useful identity

$$\frac{\delta x_a(\tau)}{\delta x_b(t)} = \delta_{ab} \delta(\tau - t) \; .$$

In terms of the functional derivative, the functional Taylor series has the following form

$$W[x + \delta x] = W[x] + \int_{t_a}^{t_b} \frac{\delta W[x]}{\delta x(t)} \delta x(t) dt + \cdots$$
$$= exp\left(\int_{t_a}^{t_b} \frac{\delta}{\delta x(t)}\right) W[x] \delta x(t) dt.$$

For functionals that have the form of an integral of an ordinary function

$$W[x] = \int_{t_a}^{t_b} F(x) \, dt \,,$$

the functional derivative of W[x] is related to the ordinary derivative dF/dx

$$\frac{\delta W[x]}{\delta x(t)} = \frac{dF(x)}{dx} \,.$$

Here are some examples:

(a)
$$F(x) = x^{3}(t), \quad W[x] = \int_{t_{a}}^{t_{b}} x^{3}(t)dt$$

(b)
$$F(x) = \sin x(t), \quad W[x] = \int_{t_a}^{t_b} \sin x(t) dt$$

(c)
$$F(x,y) = x^3(t)y^3(t), \quad W[x,y] = \int_{t_a}^{t_b} x^3(t)y^3(t)dt.$$

Here are some examples:

(a)
$$F(x) = x^{3}(t), \quad W[x] = \int_{t_{a}}^{t_{b}} x^{3}(t)dt$$

 $\frac{\delta W[x]}{\delta x(t)} = 3x^{2}(t),$
(b) $F(x) = \sin x(t), \quad W[x] = \int_{t_{a}}^{t_{b}} \sin x(t)dt$
 $\frac{\delta W[x]}{\delta x(t)} = \cos x(t),$
(c) $F(x,y) = x^{3}(t)y^{3}(t), \quad W[x,y] = \int_{t_{a}}^{t_{b}} x^{3}(t)y^{3}(t)dt$
 $\frac{\delta W[x,y]}{\delta x(t)} = 3x^{2}(t)y^{3}(t).$

1.3 Back to Hamilton's Principle

The action is defined as

$$S[x] \equiv \int_{t_a}^{t_b} L(x, \dot{x}) dt$$
$$= \int_{t_a}^{t_b} (T(x, \dot{x}) - U(x, \dot{x})) dt$$
$$= S_T - S_U,$$

with

$$S_T[x] = \int_{t_a}^{t_b} T(x, \dot{x}) \, dt \,,$$

and

$$S_U[x] = \int_{t_a}^{t_b} U(x, \dot{x}) dt.$$

Then the functional derivative of the action becomes

$$\frac{\delta S[x]}{\delta x(t)} = \frac{\delta S_T[x]}{\delta x(t)} - \frac{\delta S_U[x]}{\delta x(t)}.$$

Let's consider U = U(x) for a conserved energy. Since U(x) is an ordinary function of x,

$$\frac{\delta S_U[x]}{\delta x(t)} = \frac{dU(x)}{dx} = U'(x(t)).$$

The functional derivative of the S_T term can be evaluated from

$$S_{T}[x + \delta x] = \int_{t_{a}}^{t_{b}} \frac{1}{2}m(\dot{x} + \delta \dot{x})^{2} dt$$

= $\int_{t_{a}}^{t_{b}} \frac{1}{2}m\dot{x}^{2} dt + \int_{t_{a}}^{t_{b}} m\dot{x}\delta\dot{x} dt + O(\delta x^{2})$
= $S_{T}[x] + \int_{t_{a}}^{t_{b}} m\dot{x}\delta\dot{x} dt + O(\delta x^{2}).$

The linear term in $\delta \dot{x}$ becomes

$$\begin{split} \int_{t_a}^{t_b} m\dot{x}\delta\dot{x}\,dt &= \int_{t_a}^{t_b} m\dot{x}\frac{d}{dt}(\delta x)\,dt \\ &= \int_{t_a}^{t_b} m\frac{d}{dt}(\dot{x}\delta x)\,dt - \int_{t_a}^{t_b} m\frac{d}{dt}(\dot{x})\delta x(t)\,dt \\ &= m\dot{x}(t_b)\delta x(t_b) - m\dot{x}(t_a)\delta x(t_a) - \int_{t_a}^{t_b} m\frac{d}{dt}(\dot{x})\delta x(t)\,dt \\ &= m\dot{x}(t_b)\delta x(t_b) - m\dot{x}(t_a)\delta x(t_a) - \int_{t_a}^{t_b} m\ddot{x}\delta x(t)\,dt \,. \end{split}$$

We note that

$$\dot{x} + \delta \dot{x} = \frac{d}{dt} (x(t) + \delta x(t))$$
$$= \dot{x} + \frac{d}{dt} (\delta x(t)).$$

Therefore, we have

$$\delta \dot{x} = \frac{d}{dt} (\delta x(t)).$$

The initial conditions demand

$$x(t_a) = x_a = \text{constant}$$

 $x(t_b) = x_b = \text{constant}.$

Thus

$$\delta x(t_a) = \delta x_a = 0$$

$$\delta x(t_b) = \delta x_b = 0.$$

Now we have

$$S_T[x + \delta x] = S_T[x] - \int_{t_a}^{t_b} m\ddot{x}\delta x(t) dt$$

and so

$$\frac{\delta S_T[x]}{\delta x(t)} = -m\ddot{x}(t).$$

The extremization condition for S[x] is

$$0 = \frac{\delta S[x]}{\delta x(t)}$$
$$= \frac{\delta S_T[x]}{\delta x(t)} - \frac{\delta S_U[x]}{\delta x(t)}$$
$$= -m\ddot{x}(t) - U'(x)$$

or

$$m\ddot{x}(t) = -U'(x) = F(x),$$

which is just Newton's second law of motion.

1.4 More Degrees of Freedom

Let us consider a system with N particles moving in one dimension with coordinates x_1, x_2, \dots, x_N . The Lagrangian is

$$L = T - U = \sum_{i=1}^{N} \frac{1}{2} m_i \dot{x}_i^2 - U(x_1, x_2, \cdots, x_N),$$

where T is the total kinetic energy and U is the potential energy. It is easy to see that

$$\frac{\delta S[x]}{\delta x_i(t)} = -m_i \ddot{x}_i - U_i(x_1, \cdots, x_N) = -m_i \ddot{x}_i - \frac{\partial}{\partial x_i} U(x_1, \cdots, x_N) = F_i ,$$

and $-U_i$ is the force on particle *i*.

For S[x] to be stationary, we must have

$$\frac{\delta S[x]}{\delta x_i(t)} = -m_i \ddot{x}_i - U_i(x_1, \cdots, x_N) = 0,$$

for each *i*, which gives $F_i = m\ddot{x}_i = ma_i$ for every particle.

Kronecker delta Symbol and Dirac delta Function

The Kronecker delta symbol (δ_{ij} for discrete variables is defined as

$$\delta_{ij} = 1$$
, for $i = j$, and $\delta_{ij} = 0$, for $i \neq j$,

such that

$$\sum_{i=1}^N \delta_{ij} g_i = g_j \,.$$

The Dirac delta function for continuous variables is defined as

 $\delta(x - x_0) = \infty$, for $x = x_0$, and $\delta(x - x_0) = 0$, for $x \neq x_0$,

such that

$$\int_{x_1}^{x_2} \delta(x - x_0) f(x) \, dx = f(x_0) \,, \quad \text{for } x_1 < x_0 < x_2 \,.$$

Review of Coordinates

Cartesian Coordinates

The displacement of a particle in Cartesian coordinates is described as

 $\vec{r} = \vec{x} = x\hat{x} + y\hat{y} + z\hat{z}$

where \hat{x} , \hat{y} , \hat{y} are unit vectors.

Cylindrical Coordinates

The cylindrical coordinates are (ρ, ϕ, z) , where

$$\rho = \sqrt{x^2 + y^2}$$

and $0 \le \phi \le 2\pi$ $\phi = \tan^{-1}\left(\frac{y}{x}\right)$, for x > 0, and $\phi = -\sin^{-1}\left(\frac{y}{x}\right) + \pi$, for x < 0.

Spherical Coordinates

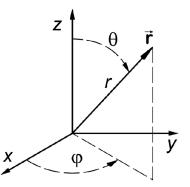


Figure 1: Spherical coordinates

The spherical coordinates are (r, θ, ϕ) , where

$$r = \sqrt{x^2 + y^2 + z^2}$$
, and $\theta = \cos^{-1}\left(\frac{z}{r}\right)$,

with
$$0 \le \theta \le \pi$$
 and $0 \le \phi \le 2\pi$
 $\phi = \tan^{-1}\left(\frac{y}{x}\right)$, for $x > 0$, and $\phi = -\sin^{-1}\left(\frac{y}{x}\right) + \pi$, for $x < 0$.

1.5 The Euler-Lagrange equation

The action (S) is defined as

$$S[q] \equiv \int_{t_a}^{t_b} L(q, \dot{q}) dt \,.$$

The Lagrangian (L) is defined as the difference of the kinetic energy (T) and the potential energy (U), $L(q, \dot{q}) \equiv T(q, \dot{q}) - U(q, \dot{q})$, and it is a function of generalized coordinates (q_i) and time derivatives of the generalized coordinates (\dot{q}_i) , where q can be a vector with components $q_i, i = 1, 2, \dots, N$.

The functional derivative of the action S[q] with respect to $q_i(t)$ is

$$\frac{\delta S[q]}{\delta q_i(t)} = \frac{\partial L(q, \dot{q})}{\partial q_i(t)} - \frac{d}{dt} \left[\frac{\partial L(q, \dot{q})}{\partial \dot{q}_i(t)} \right]$$

The first term arises from the Taylor expansion of the $q_i(t)$ dependence; the second term arises from the Taylor expansion of the $\dot{q}_i(t)$ followed by an integration by parts which gives the minus sign. In one dimension with q(t) = x(t), we have

$$\begin{split} S[x + \delta x] &= \int_{t_a}^{t_b} L(x + \delta x, \dot{x} + \delta \dot{x}) \, dt \\ &= \int_{t_a}^{t_b} \left[L(x, \dot{x}) + \delta x \frac{\partial L}{\partial x} + \delta \dot{x} \frac{\partial L}{\partial \dot{x}} \right] \, dt + O(\delta x^2) \\ &= S[x] + \int_{t_a}^{t_b} \left[\delta x \frac{\partial L}{\partial x} + \frac{d}{dt} (\delta x \frac{\partial L}{\partial \dot{x}}) - \delta x \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \, dt + O(\delta x^2) \\ &= S[x] + \int_{t_a}^{t_b} \left[\delta x \frac{\partial L}{\partial x} - \delta x \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \, dt + \left[\delta x \frac{\partial L}{\partial \dot{x}} \right]_{t_a}^{t_b} + O(\delta x^2) \\ &= S[x] + \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \, \delta x \, dt + O(\delta x^2), \end{split}$$

where $\delta x(t_a) = 0 = \delta x(t_b)$ since x_a and x_b are fixed end points.

We have just found

$$S[x + \delta x] = S[x] + \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \delta x \, d\tau + O(\delta x^2) \,.$$

The functional derivative can be defined as the coefficient of the linear term in $\delta x(t)$: $\delta S[x]/\delta x(t) = \partial L/\partial x(t) - d/dt[\partial L/\partial \dot{x}(t)]$, and it should be derived as

$$\begin{split} \frac{\delta S[x]}{\delta x(t)} &\equiv \lim_{\delta x \to 0} \frac{S[x + \delta x] - S[x]}{\delta x(t)} \\ &= \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \frac{\delta x(\tau)}{\delta x(t)} d\tau \\ &= \int_{t_a}^{t_b} \left[\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} \right] \delta(\tau - t) d\tau \\ &= \frac{\partial L}{\partial x(t)} - \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{x}(t)} \right] \,. \end{split}$$

If S[x] is stationary, the functional derivative with respect to x(t) must vanish, i.e.

$$\frac{\delta S[x]}{\delta x(t)} = \frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = 0.$$

N.B. The Hamilton's principle implies that the solution for the motion along the classical path with stationary action satisfies

$$\frac{\partial L}{\partial x} - \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} = 0.$$

which is called the Euler-Lagrange equation. If x or q has several components, the Euler-Lagrange equation must be true for each component (q_i) separately:

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \left[\frac{\partial L}{\partial \dot{q}_i} \right] = 0 \,.$$

Example: A Frictionless Table

Let's consider a frictionless table in the x - y plane with a hole at the origin. A mass m_1 slides on the surface of the table but it is attached to a massless string of length ℓ that goes through the hole at the center of the table and hangs straight down where it is attached to a mass m_2 .

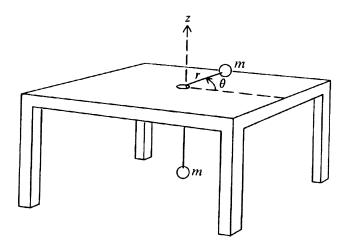


Figure 2: Frictionless table.

This system can be described by the length r of the string on the table and the angle θ of the string on the table from the x axis. The kinetic energy is

$$T(r, \dot{r}, \theta, \dot{\theta}) = \frac{1}{2}(m_1 + m_2)\dot{r}^2 + \frac{1}{2}m_1r^2\dot{\theta}^2,$$

where the first term is the kinetic energy of translation and the second term is the kinetic energy of rotation.

The gravitational potential energy is

 $U(r) = m_2 gr,$

such that $U(r=0) = 0 = U_{\min}$ and $U(r=\ell) = m_2 g \ell = U_{MAX}$. The Lagrangian is

$$L(r, \dot{r}, \theta, \dot{\theta}) = T - U$$

= $\frac{1}{2}(m_1 + m_2)\dot{r}^2 + \frac{1}{2}m_1r^2\dot{\theta}^2 - m_2gr.$

The Euler-Lagrange equations are

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0.$$

The Lagrangian is

$$L(r, \dot{r}, \theta, \dot{\theta}) = \frac{1}{2}(m_1 + m_2)\dot{r}^2 + \frac{1}{2}m_1r^2\dot{\theta}^2 - m_2gr.$$

The Euler-Lagrange equations are

$$\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} = 0.$$

For q = r, the equation of motion is

$$\frac{\partial L}{\partial r} - \frac{d}{dt} \frac{\partial L}{\partial \dot{r}} = 0$$
$$m_1 r \dot{\theta}^2 - m_2 g - (m_1 + m_2) \ddot{r} = 0.$$

For $q = \theta$, the equation of motion is

$$\frac{\partial L}{\partial \theta} - \frac{d}{dt} \frac{\partial L}{\partial \dot{\theta}} = 0$$

$$-\frac{d}{dt} (m_1 r^2 \dot{\theta}) = 0, \quad \text{i.e.} \quad p_{\theta} \equiv \frac{\partial L}{\partial \dot{\theta}} = m_1 r^2 \dot{\theta} = \text{ constant}.$$