

# Quantum Physics

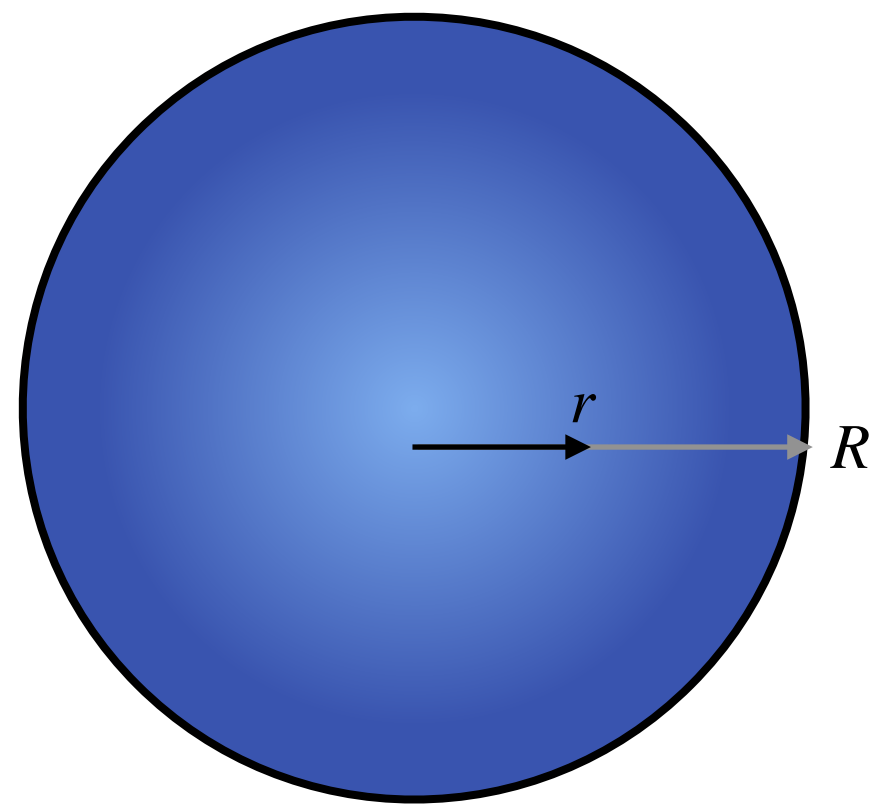
## 2024

The Theory/Framework Of *Almost* Everything *Today*

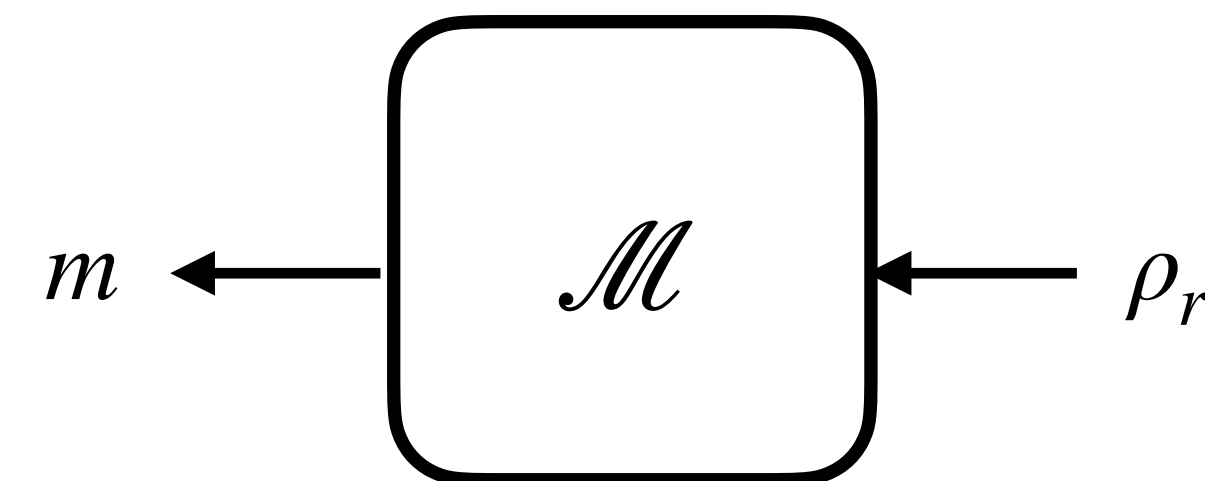
Yury Deshko

# Functionals

## And Their Use in Physics



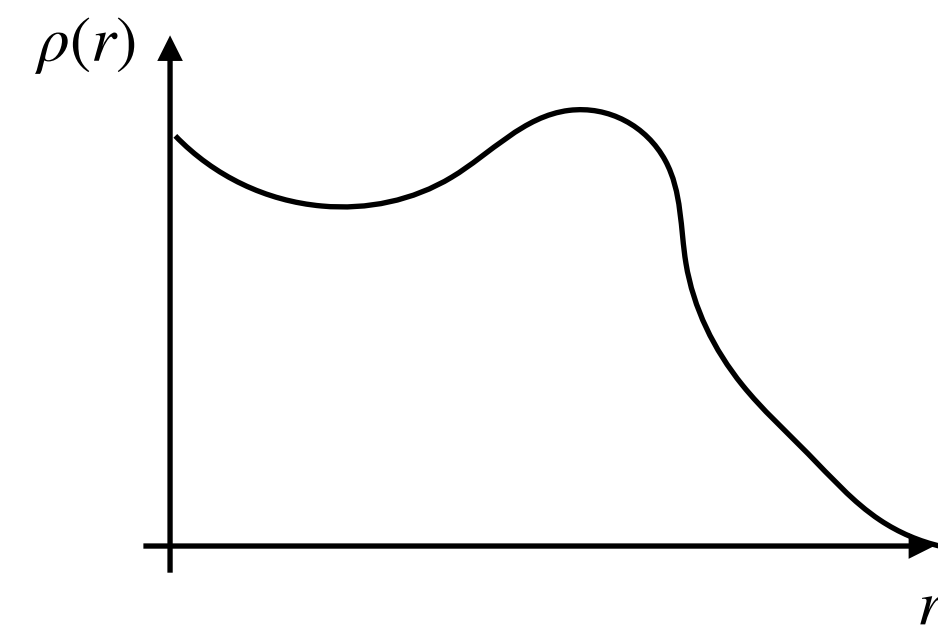
Calculate total mass for a given density distribution



$\mathcal{M}$  : **function**  $\longrightarrow$  **number**

$\rho_r$

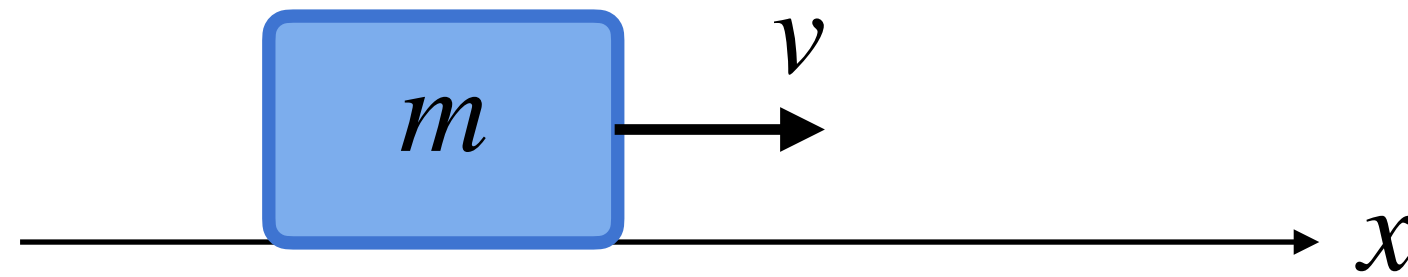
$m$



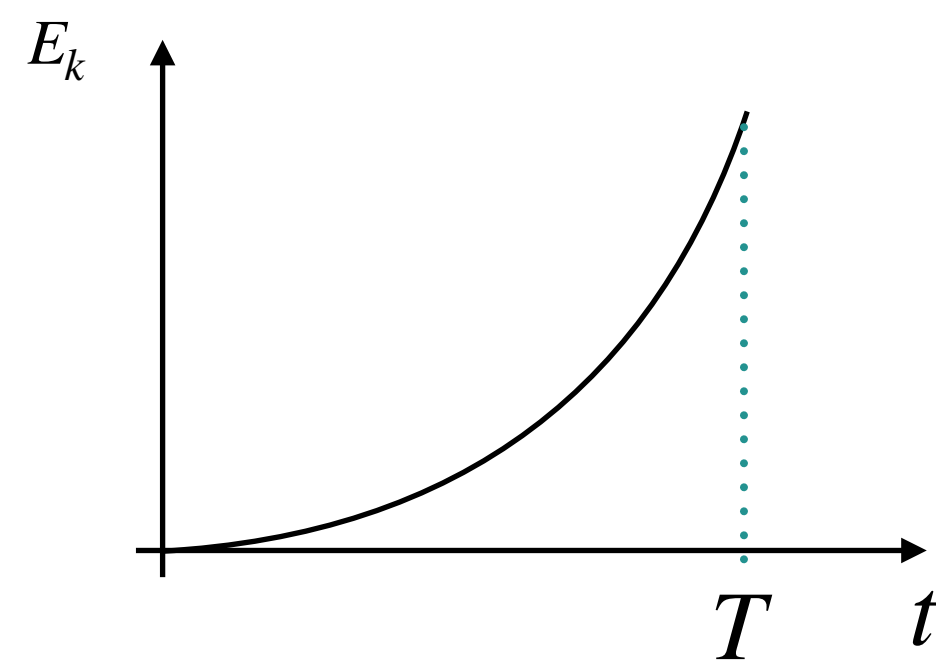
Density of a star/planet vs the radius from the center

# Functionals

## And Their Use in Physics

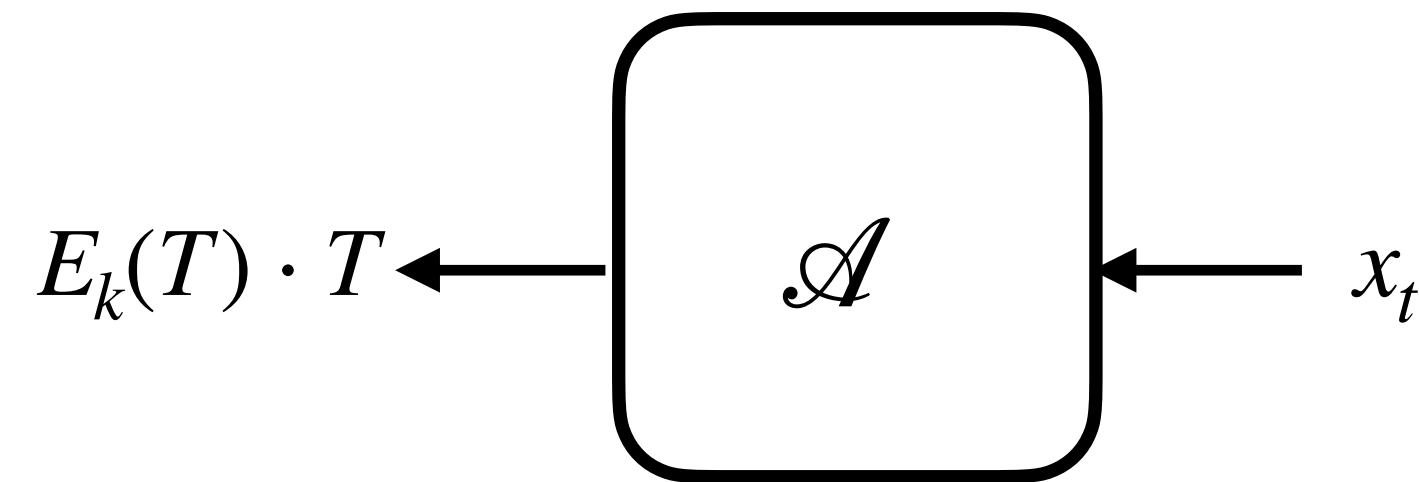


$$x_t \rightarrow v_t = \partial_t x \rightarrow E_k = \frac{mv^2}{2}$$



Kinetic energy vs time

Calculate total “action” — energy\*time



$\mathcal{A} : \text{function} \rightarrow \text{number}$

$x_t$

$E_k(T) \cdot T$

Action  $A = Et$  is of fundamental importance.

It is quantized, like electric charge  $q_e = e$

Exercise: Show that for constant acceleration,  $E_k t = px$

# Course Overview

## Course Structure And Goals

- Part 1 : Mathematical Concepts And Tools
- Part 2 : Classical Physics
- Part 3 : Quantum Physics

We want to understand SchrEq

$$\text{Operator} \longleftarrow i\hbar\partial_t |\Psi\rangle = \hat{H} |\Psi\rangle \longrightarrow \text{Vector, but can be also made an operator}$$

$\downarrow$                        $\downarrow$

Rate of change with respect to time      Operator

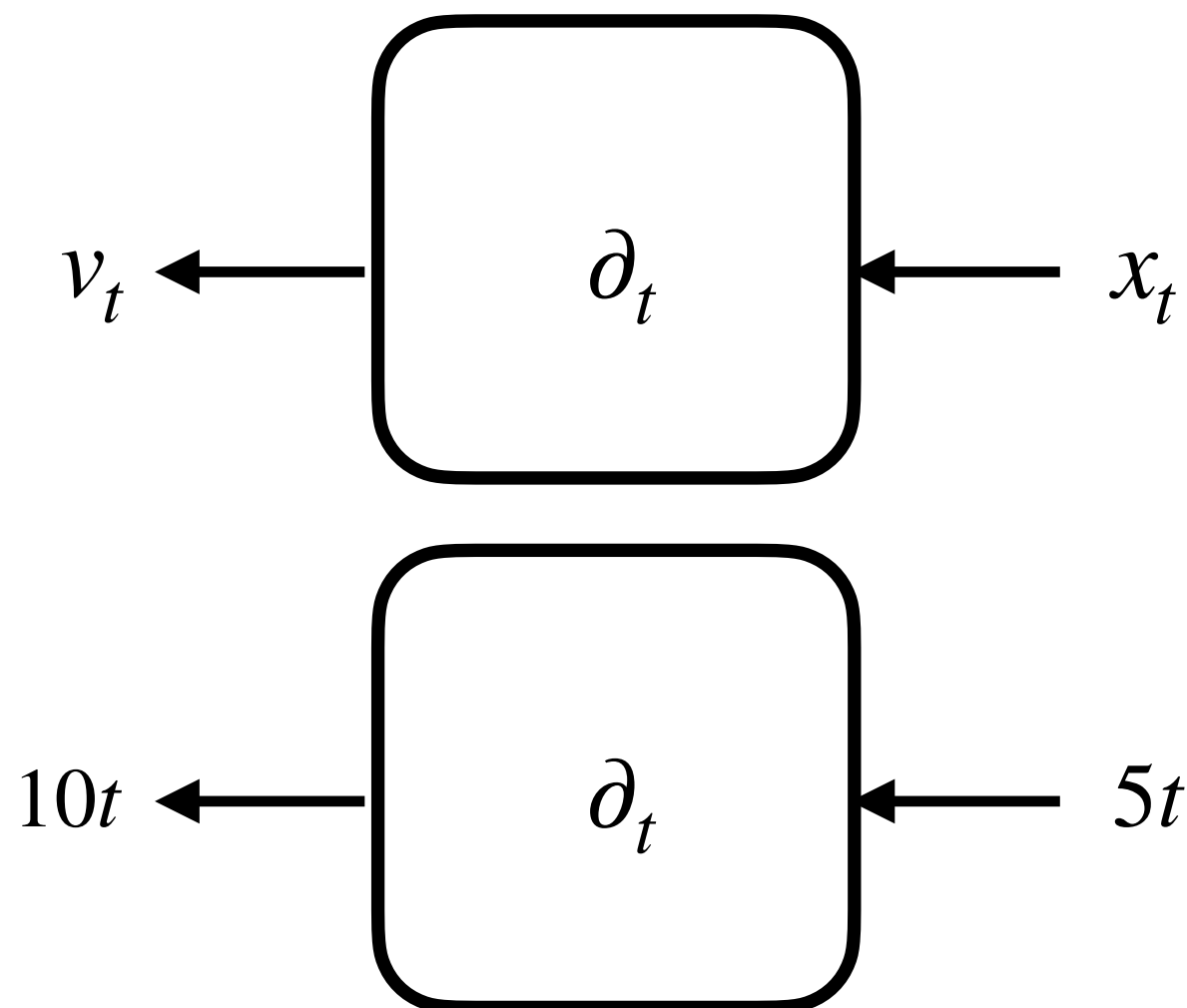
Today we will understand  $|\Psi\rangle$ .

# Warm Up

## Rate of Change Operator

$$i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle$$

Rate of change with respect to time



Function in — function out

$$x_t = \frac{at^2}{2}$$

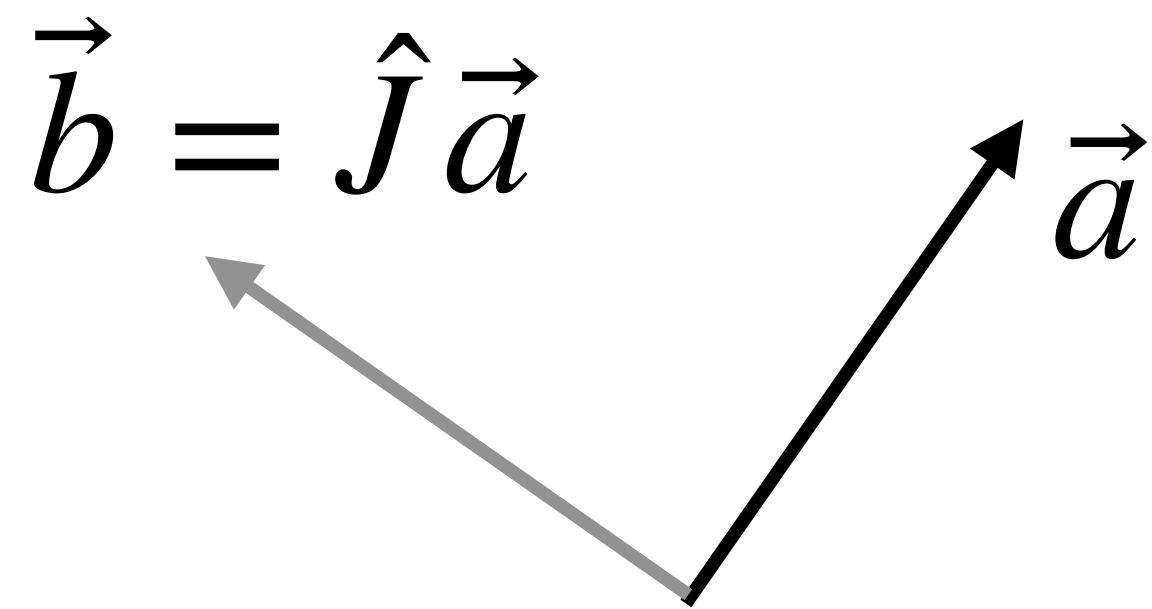
$$\delta x = 5(t + \delta t)^2 - 5t^2 = 5t^2 + 10t\delta t + 5(\delta t)^2 - 5t^2 = 10t\delta t + 5(\delta t)^2$$

$$v_t = \partial_t x = \frac{\delta x}{\delta t} = 10t + 5\delta t \approx 10t$$

$5\delta t$  is an important term, tells us about the error of real-world approximations, e.g. in numerical computations using machines, like computers.

# Special Operator

Simple Yet Powerful Orthogonal Transformation



$\hat{J}$  performs counter-clockwise rotation of any arrow.

$$\vec{b} = \hat{J} \vec{a}$$

$$\vec{c} = \hat{J} \vec{b} = \hat{J}(\hat{J} \vec{a}) = (\hat{J} \circ \hat{J}) \vec{a} = \hat{J}^2 \vec{a} = -\vec{a}$$

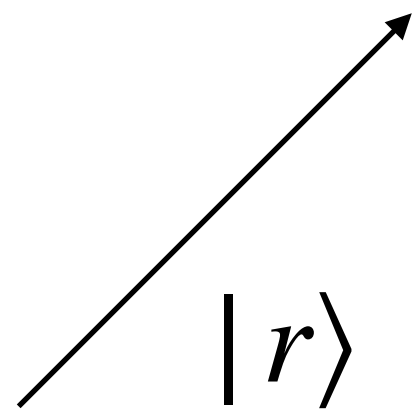
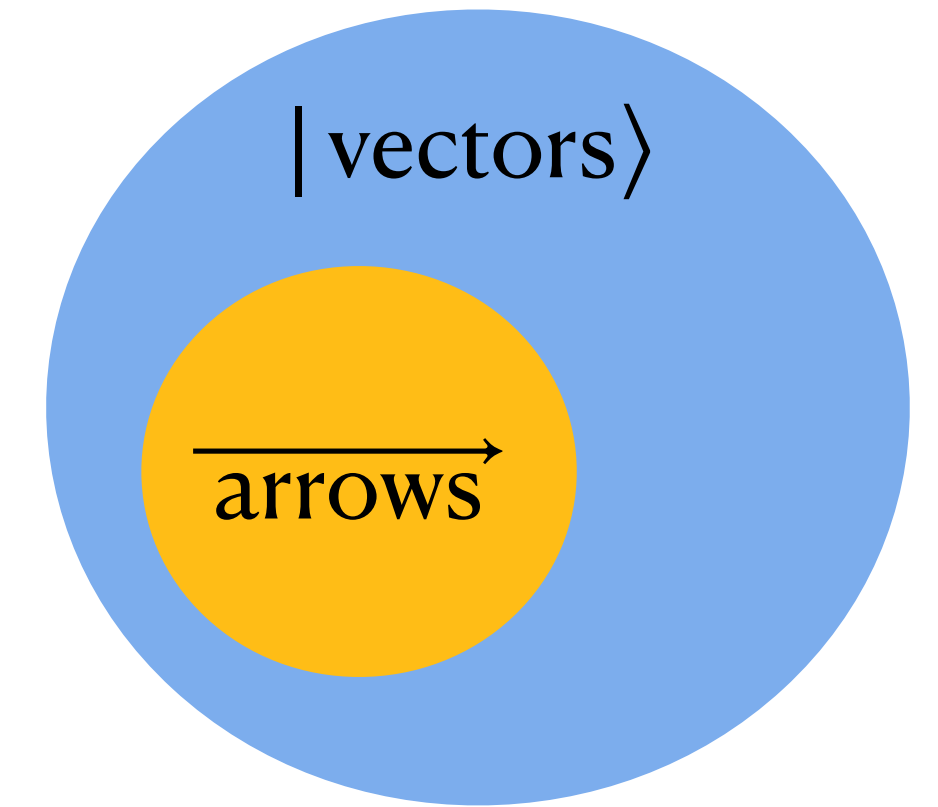
$$\hat{J}^2 = -\hat{I}$$

$$\hat{J}^3 = -\hat{J}$$

$$\hat{J}^4 = \hat{I}$$

# Dirac Notation

## Vectors are Richer Than Just Arrows



$$\vec{r} \quad \leftrightarrow \quad |r\rangle$$

$$\vec{v} \quad \leftrightarrow \quad |v\rangle$$

$$\overrightarrow{F} \quad \leftrightarrow \quad |F\rangle$$

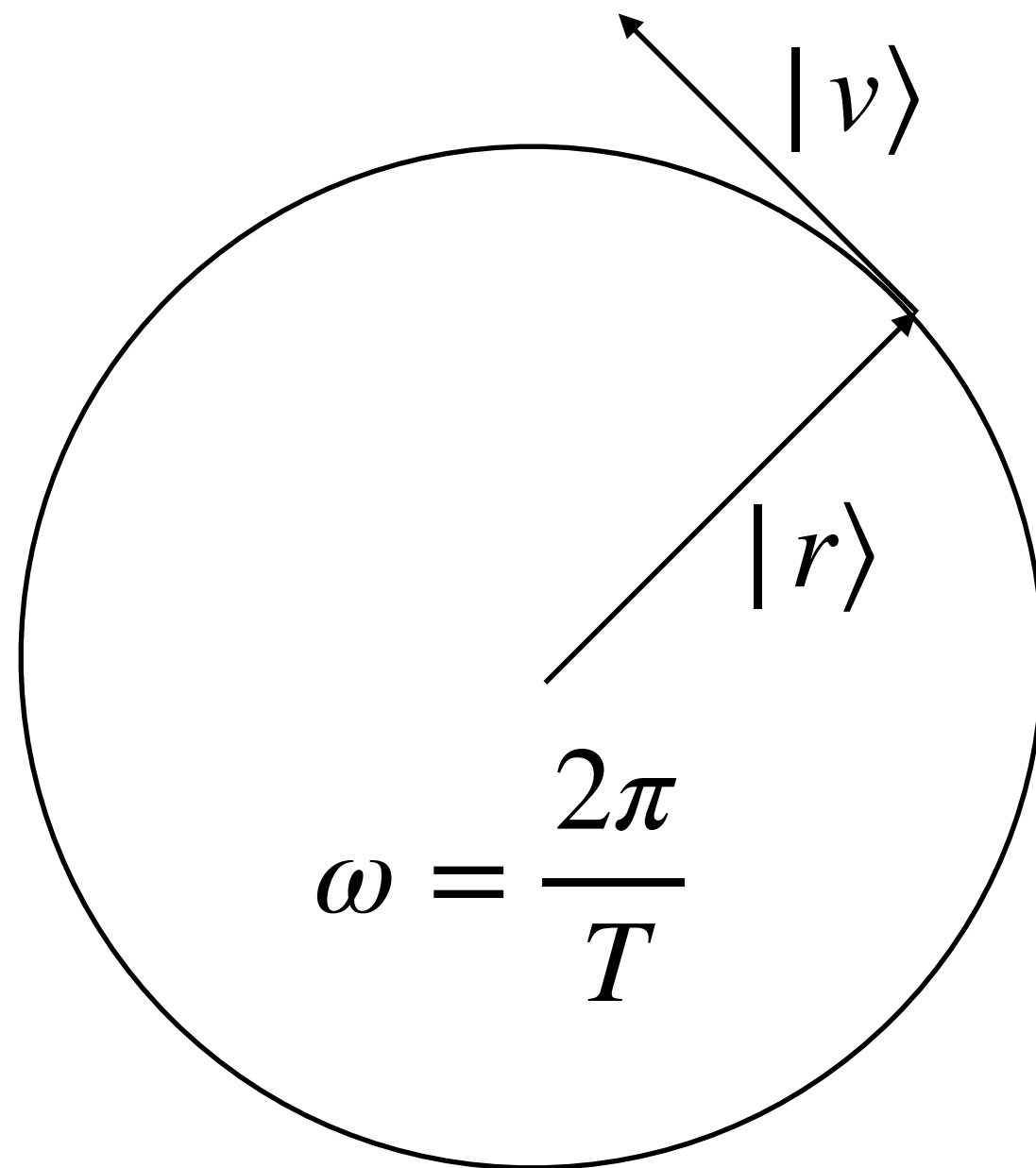
Paul Adrien Maurice Dirac in 1939 introduced modern vector notation for quantum mechanics.

$$\vec{a} \quad \leftrightarrow \quad |a\rangle$$

We can use it in “normal” physics too, if we want. Let’s switch to Dirac notation as early as possible.

# Circular Motion

## And Schrödinger Equation



Circular motion with constant angular speed  $\omega$

$$v = \frac{2\pi r}{T} = \omega r$$

$$t \rightarrow t + \delta t$$

$$|r\rangle \rightarrow |r\rangle + \delta |r\rangle \quad \delta |r\rangle \perp |r\rangle$$

$$|v\rangle = \partial_t |r\rangle \quad |v\rangle \perp |r\rangle$$

Take  $|r\rangle$ , scale it down to unit length (dividing by its length  $r$ ), then rotate with  $\hat{J}$  to make it perpendicular to  $|r\rangle$ . Finally, scale it up to the length of  $|v\rangle$  given by  $v = \omega r$

$$|v\rangle = v \hat{J} \left( \frac{1}{r} |r\rangle \right) = \omega \hat{J} |r\rangle$$

$$\partial_t |r\rangle = \omega \hat{J} |r\rangle$$

Now act with  $\hat{J}$  on both sides

$$\hat{J} \partial_t |r\rangle = -\omega |r\rangle$$

Compare to SchrEq

$$\hat{J} \hbar \partial_t |r\rangle = -\hbar \omega |r\rangle$$

$$i \hbar \partial_t |\Psi\rangle = \hat{H} |\Psi\rangle$$



# Sidenote: Special Equation

Rate of change of  $F$  is proportional to  $F$

$$\hat{J}\hbar\partial_t|r\rangle = -\hbar\omega|r\rangle$$

← Circular motion

$$i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle$$

← Quantum “motion”

$$\partial_t|r\rangle = \hat{J}\omega|r\rangle$$

$$\partial_t|\Psi\rangle = -\frac{i}{\hbar}\hat{H}|\Psi\rangle$$

$$\partial_t f = C f$$

Special case:

$$\partial_t f = f$$

“Mega”-function, one of the most powerful functions in applied math

HW: Review properties of  $a^x$ .

# State

## Physical Systems

## Basic Notion of Physics

Mathematical/symbolic expression of **state**

$$i\hbar\partial_t |\Psi\rangle = \hat{H} |\Psi\rangle$$

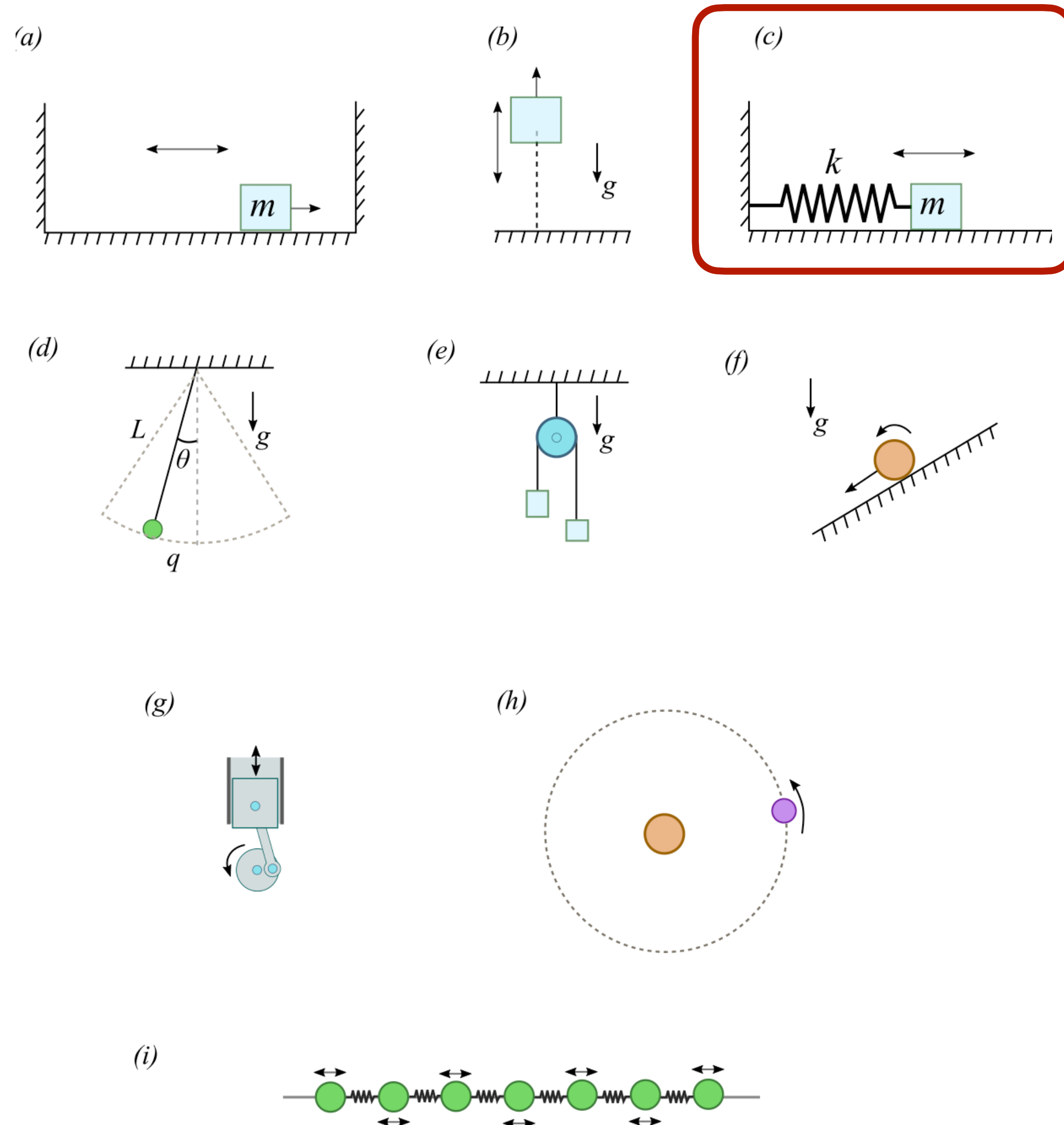
Physics studies the world. To simplify, parts of the world are isolated and studied separately.

**System** — part of the world that can be isolated and studied.

Goals of physics are

- **Describe** behavior of a system (D)
- **Explain** behavior of a system (E)
- **Predict** behavior of a system (P)

**State** — all *information*/knowledge we need to (D+P). A *complete* description of the system. All there is to know about a system at a given moment.



Describe:  $x, v$

$$E_k = mv^2/2$$

$$F = f(x, v)$$

$$a = F/m$$

$$L = mvx$$

# State

## State Evolution

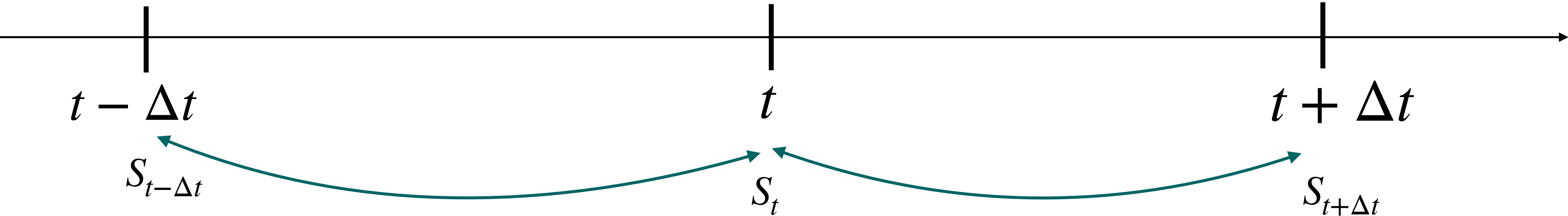
Explanation needs rules that connect “forces” to acceleration — dynamical laws:  $v = \partial_t x, a = F/m$

Describe:

$x, v, \underline{a}, \underline{F}, \underline{E_k}, \underline{E_p}, \underline{L}$

Predict:  $\partial_t S$

State



**Predict:** If we know everything about the system now (time  $t$ ) then we can find everything about the system later (time  $t + \Delta t$ ) or earlier ( $t - \Delta t$ ). *Know state now — know state at any time.*

$$\partial_t S = \hat{D} S$$

$$i\hbar \partial_t |\Psi\rangle = \hat{H} |\Psi\rangle$$

Equation of state *evolution* or state *dynamics* (how state changes in time).

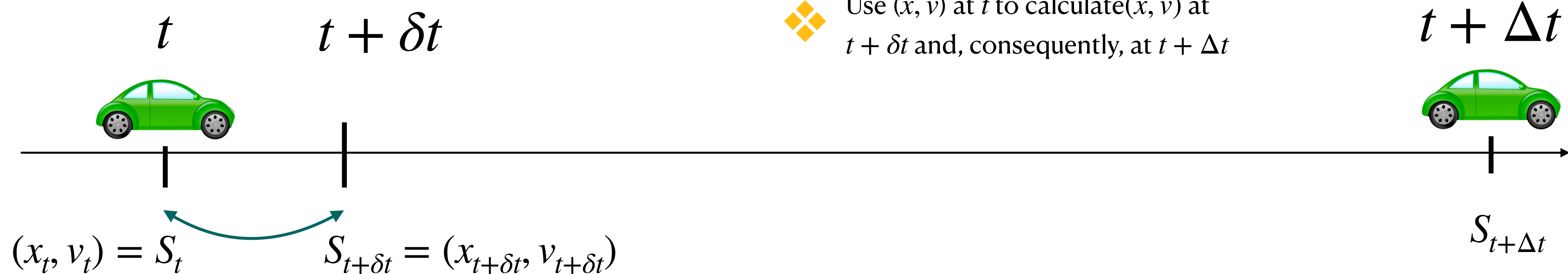
How state changes in time depends on “forces” (in  $\hat{D}$ ) and state.

# State Evolution in Newtonian Dynamics

## Basic Idea

❖ Use  $(x, v)$  to calculate everything important **now** (time  $t$ ):  
 $E_k = mv^2/2, F = f(x, v), a = F/m, L = mvx$

❖ Use  $(x, v)$  at  $t$  to calculate  $(x, v)$  at  $t + \delta t$  and, consequently, at  $t + \Delta t$

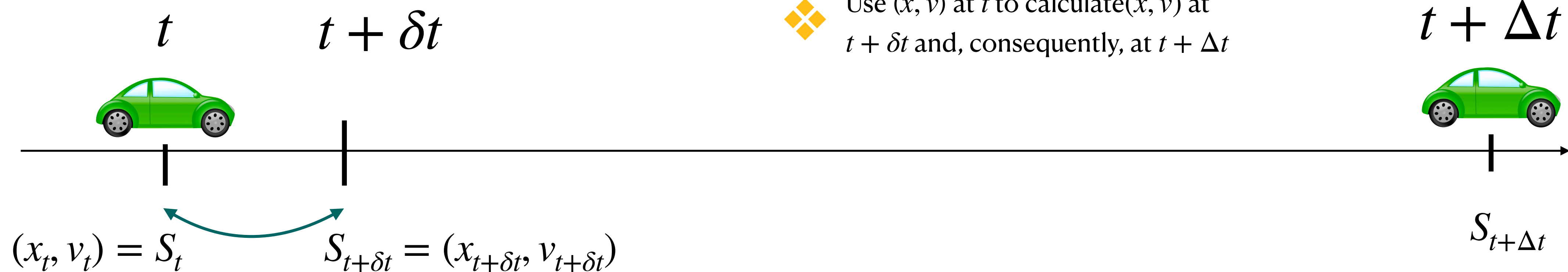


# State Evolution in Newtonian Dynamics

## Basic Idea

❖ Use  $(x, v)$  to calculate everything important **now** (time  $t$ ):  
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❖ Use  $(x, v)$  at  $t$  to calculate  $(x, v)$  at  $t + \delta t$  and, consequently, at  $t + \Delta t$



$$x_{t+\delta t} = x_t + v_t \delta t$$

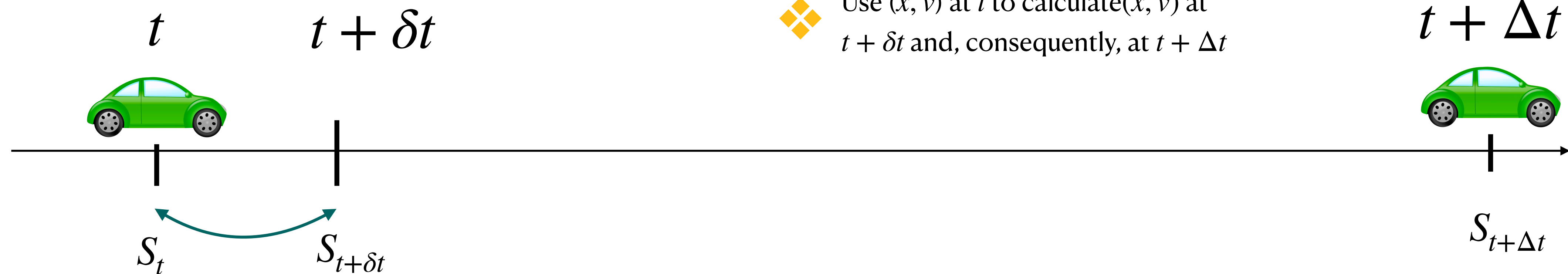
$$v_{t+\delta t} = v_t + a_t \delta t$$

# State Evolution in Newtonian Dynamics

## Basic Idea

❖ Use  $(x, v)$  to calculate everything important **now** (time  $t$ ):  
 $E_k = mv^2/2, F = f(x, v), a = F/m, L = mvx$

❖ Use  $(x, v)$  at  $t$  to calculate  $(x, v)$  at  $t + \delta t$  and, consequently, at  $t + \Delta t$



$$x_{t+\delta t} = x_t + v_t \delta t$$

$$v_{t+\delta t} = v_t + a_t \delta t$$

$a_{t+\delta t} = a_t + b_t \delta t$

 $ma_t = F_t \text{ and } F = f(x, v)$

$$F = kx \quad \text{— Hooke's law}$$

$$F = \frac{A}{x^2} \quad \text{— Newton's gravitation or Coulomb's law}$$

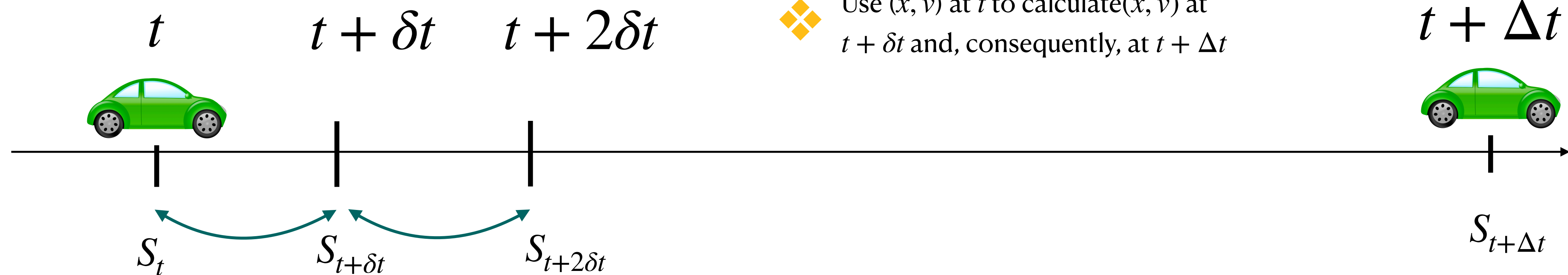
$$F = Bv \quad \text{— Lorentz force}$$

# State Evolution in Newtonian Dynamics

## Basic Idea

❖ Use  $(x, v)$  to calculate everything important **now** (time  $t$ ):  
 $E_k = mv^2/2, F = f(x, v), a = F/m, L = mvx$

❖ Use  $(x, v)$  at  $t$  to calculate  $(x, v)$  at  $t + \delta t$  and, consequently, at  $t + \Delta t$



$$x_{t+\delta t} = x_t + v_t \delta t$$

$$v_{t+\delta t} = v_t + a_t \delta t$$

$$\cancel{a_{t+\delta t} = a_t + b_t \delta t} \quad ma_t = F_t \text{ and } F = f(x, v)$$

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$$F = Bv \quad \text{— Lorentz force}$$

State in Newtonian mechanics:  $S_t = (x, v)$



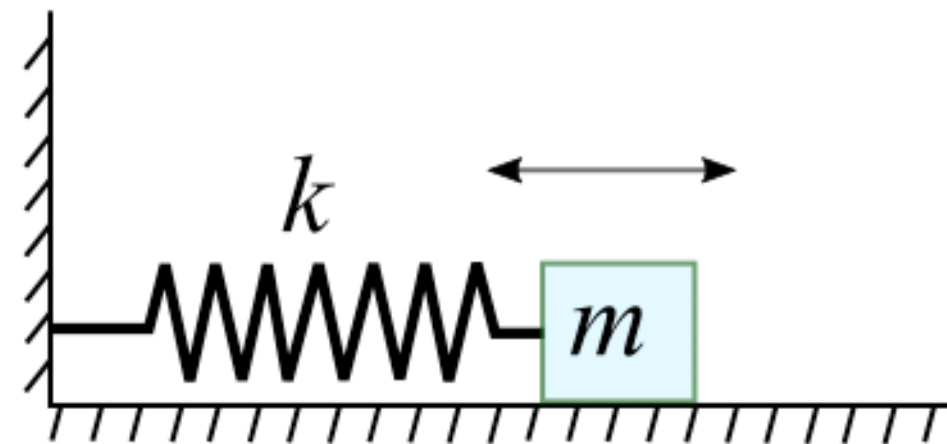
# State Evolution in Newtonian Dynamics

## Harmonic Oscillator Example

State in Newtonian mechanics:  $S_t = (x, v)$

$$x_{t+\delta t} = x_t + v_t \delta t$$

$$v_{t+\delta t} = v_t + a_t \delta t$$



$$x_0 \rightarrow x_t$$

$$v_0 \rightarrow v_t$$

$$S_0 \rightarrow S_t$$

$$\begin{aligned} \partial_t x &= v \\ \partial_t v &= F/m \end{aligned} \rightarrow \partial_t S = ?$$

How to combine two equations into one for state  $S$ ?

One solution: Make  $x$  and  $v$  parts/components of some vector  $|\xi\rangle = (x, v)$

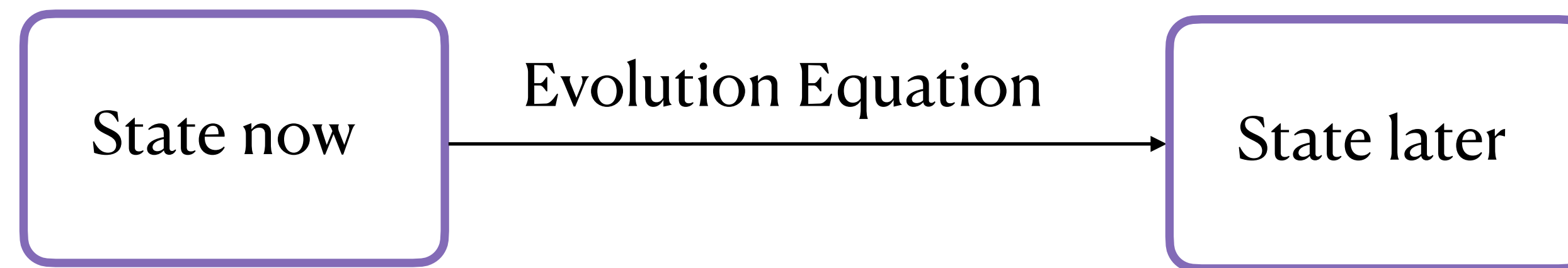
Study the script with numerical calculations.



# Determinism

## General Concept

Given initial state  $S_0$  all later states  $S_t$  are uniquely determined. Nothing random.



The equation  $\partial_t S = \hat{D} S_t$  is a symbolic expression of a *deterministic* evolution of state.

$$S_{t+\delta t} = S_t + \delta t \cdot (\partial_t S) = S_t + \delta t \hat{D} S_t$$

$$S_{t+\delta t} = (\hat{I} + \delta t \hat{D}) S_t$$

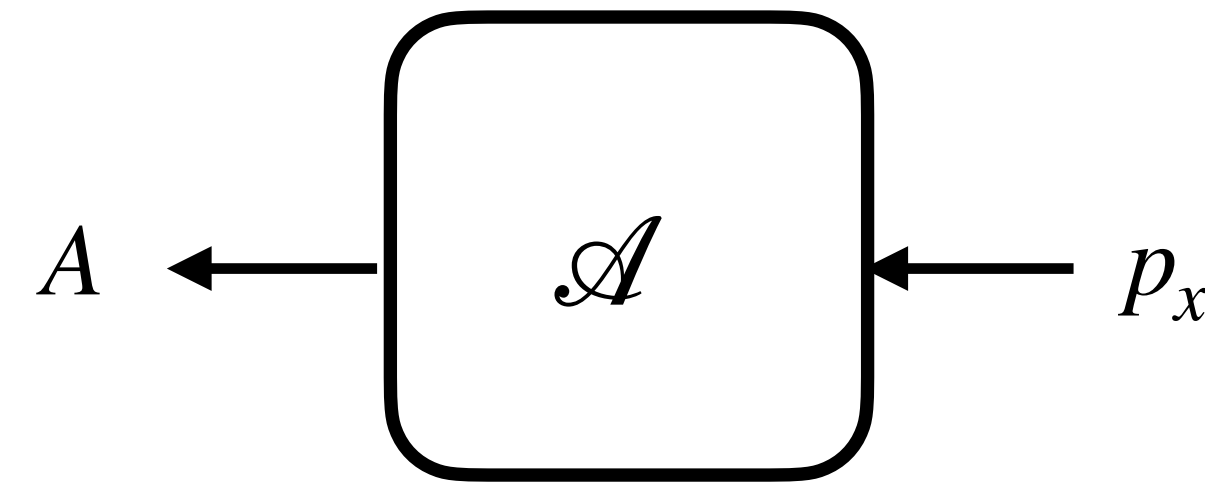
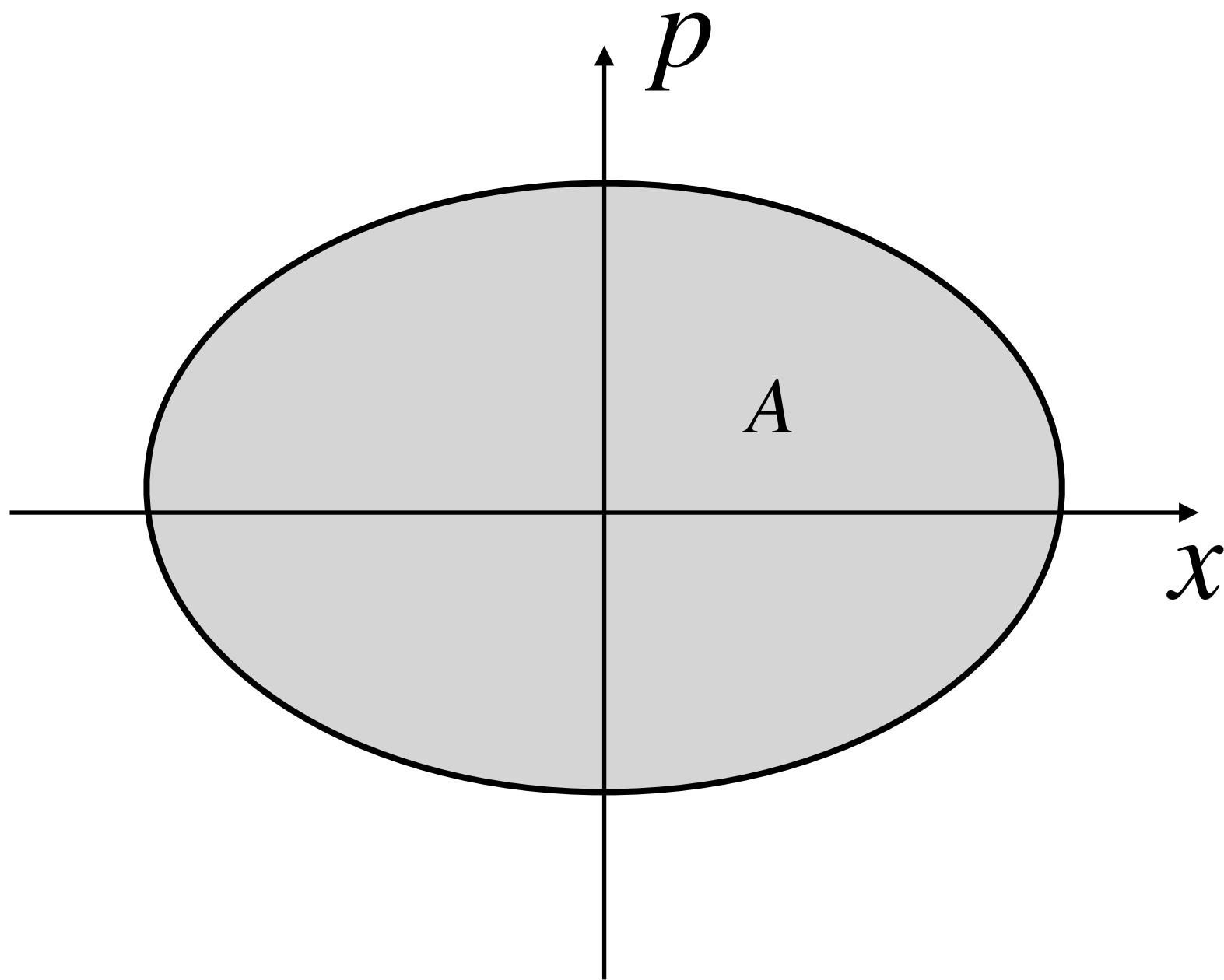
$$S_{t+2\delta t} = (\hat{I} + \delta t \hat{D}) S_{t+\delta t} = (\hat{I} + \delta t \hat{D})^2 S_t$$

$$S_{t+\Delta t} = (\hat{I} + \delta t \hat{D})^N S_t \quad N = \Delta t / \delta t$$

# Functionals

## Very Important Functional: Action

Calculate total area of the figure in phase space.



$\mathcal{A} : \text{function} \rightarrow \text{number}$

Works for confined motion only.

# Functionals

## Very Important Functional: Action

$$x_t \rightarrow v_t = \partial_t x$$

$$E_k = \frac{mv_t^2}{2}$$

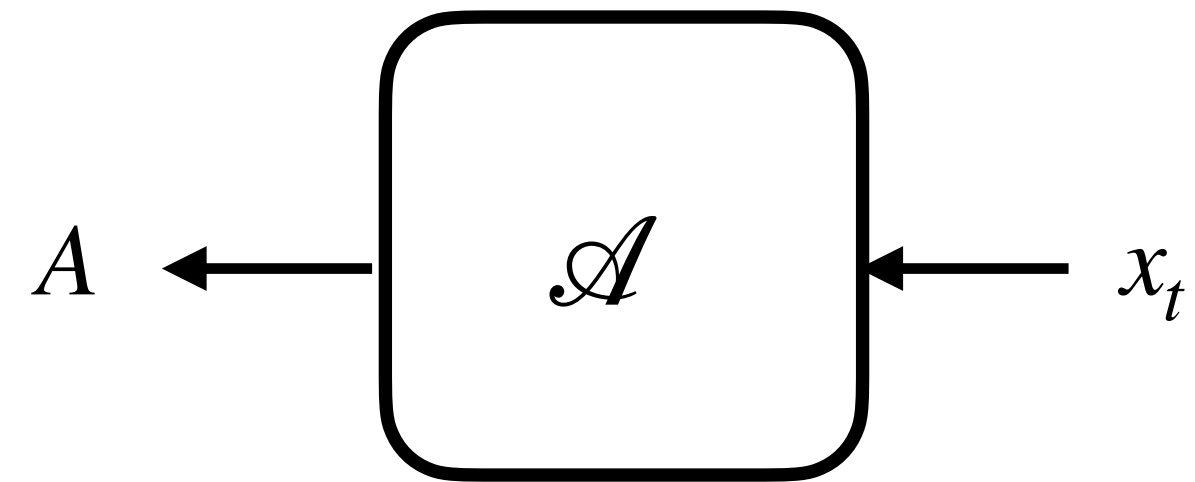
$$E_p = \frac{kx_t^2}{2}$$

$$L_t = E_k - E_p$$

$$\delta A = L \delta t$$

$$A = \int \delta A$$

Calculate total imbalance of kinetic energy over potential energy accumulated during the motion

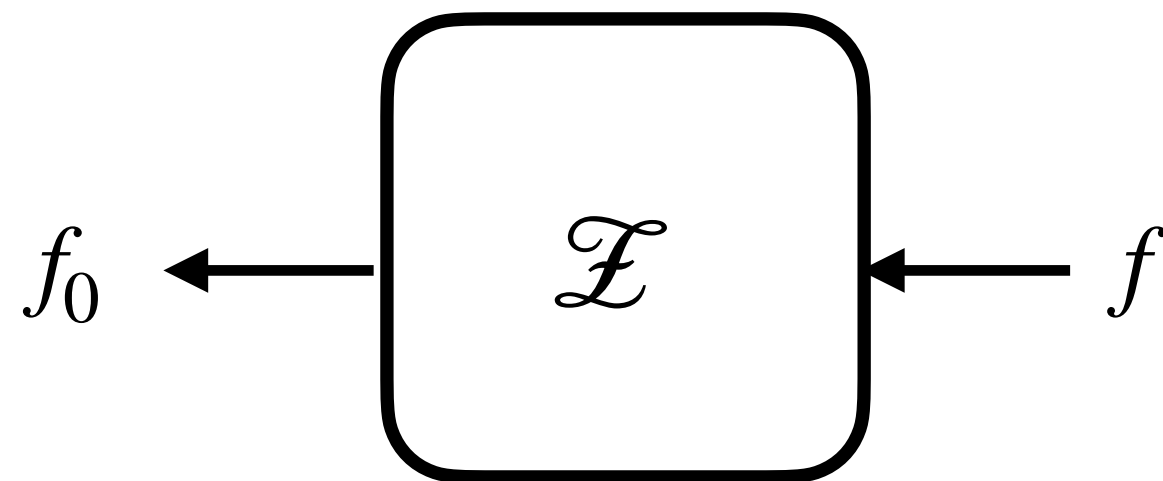


$\mathcal{A}$  : **function**  $\longrightarrow$  **number**

# Functionals

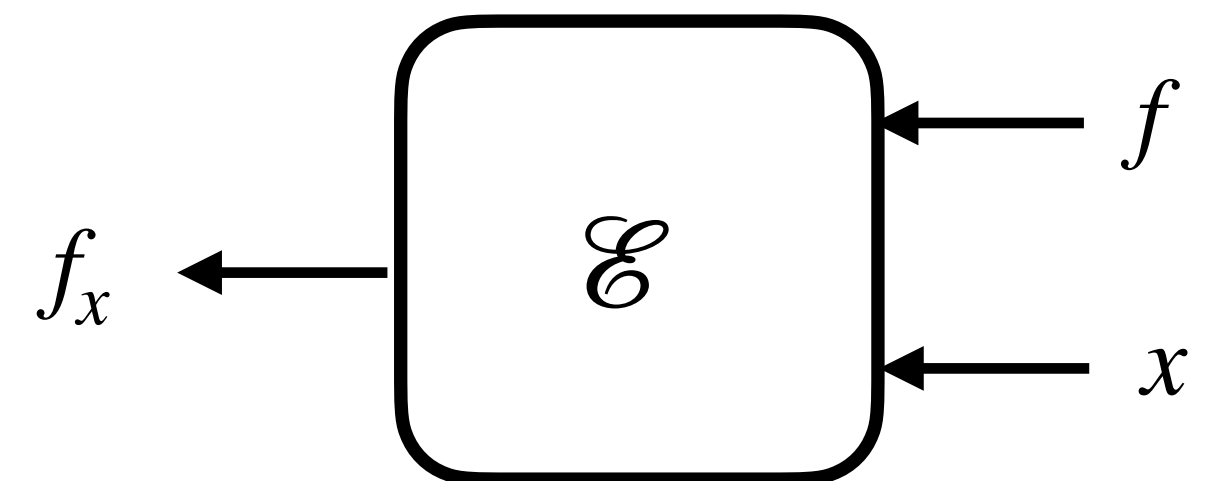
## Function Application

Evaluate function at zero



$\mathcal{L} : \text{function} \longrightarrow \text{number}$

Evaluate function at a given point



$\mathcal{E} : \text{function and number} \longrightarrow \text{number}$

$$\mathcal{E} f x = f \mathcal{E} x = f(x) = f x$$

$$\partial t f = \partial_t f$$

Sin of dropping infix operator:  $3xy = 3 \times x \times y$

# Self-Test

**Answer These Questions 1hr After Class**

1. What is an operator and why  $\partial_t$  is an operator?
2. What is Dirac notation?
3. What do circular motion and Schrödinger equation have in common?
4. What is a system?
5. What is a state?
6. What are three main goals of physics?
7. What is determinism?
8. How is the equation for rate of change of state in time called?

# Homework Problems

## Mathematical Concepts and Notation Day 3

- Review the properties of the function  $a^x$ .
- Solve the equation  $x^3 + x^2 + x + 1 = 0$  in terms of real numbers.
- Evaluate  $\hat{J}^3 + \hat{J}^2 + \hat{J} + \hat{I}$ .
- Consider the “flipping” operator  $\hat{F} = -\hat{I}$ . Evaluate  $\hat{F}^3 + \hat{F}^2 + \hat{F} + \hat{I}$ .
- Consider the operator of 90-degree rotation clock-wise:  $\hat{G}$ . How is it related to  $\hat{J}$  and  $\hat{F}$ ?
- Evaluate  $\hat{G}^3 + \hat{G}^2 + \hat{G} + \hat{I}$
- **Challenge and fun:** Express  $\frac{1}{1 - \hat{J}/2}$  in terms of  $\hat{I}$  and  $\hat{J}$ .
- Play with the script: Add friction, change computation method to use energy conservation, use non-linear formulas for  $\delta x$ .

# Quantum Theory

## In a Nutshell

### II. POSTULATES FOR QUANTUM MECHANICS

In this paper, all **state vectors** are supposed to be **normalized**, and **mixed states** are represented by **density operators** i.e., **positive operators with unit trace**. Let  $A$  be an **observable** with a **nondegenerate purely discrete spectrum**. Let  $\phi_1, \phi_2, \dots$  be a **complete orthonormal sequence of eigenvectors of  $A$**  and  $a_1, a_2, \dots$  the corresponding **eigenvalues**; by assumption, all different from each other.

According to the standard formulation of quantum mechanics, on the result of a measurement of the observable  $A$  the following postulates are posed:

(A1) *If the system is in the **state  $\psi$**  at the time of measurement, the eigenvalue  $a_n$  is obtained as the outcome of measurement with the **probability  $|\langle \phi_n | \psi \rangle|^2$***

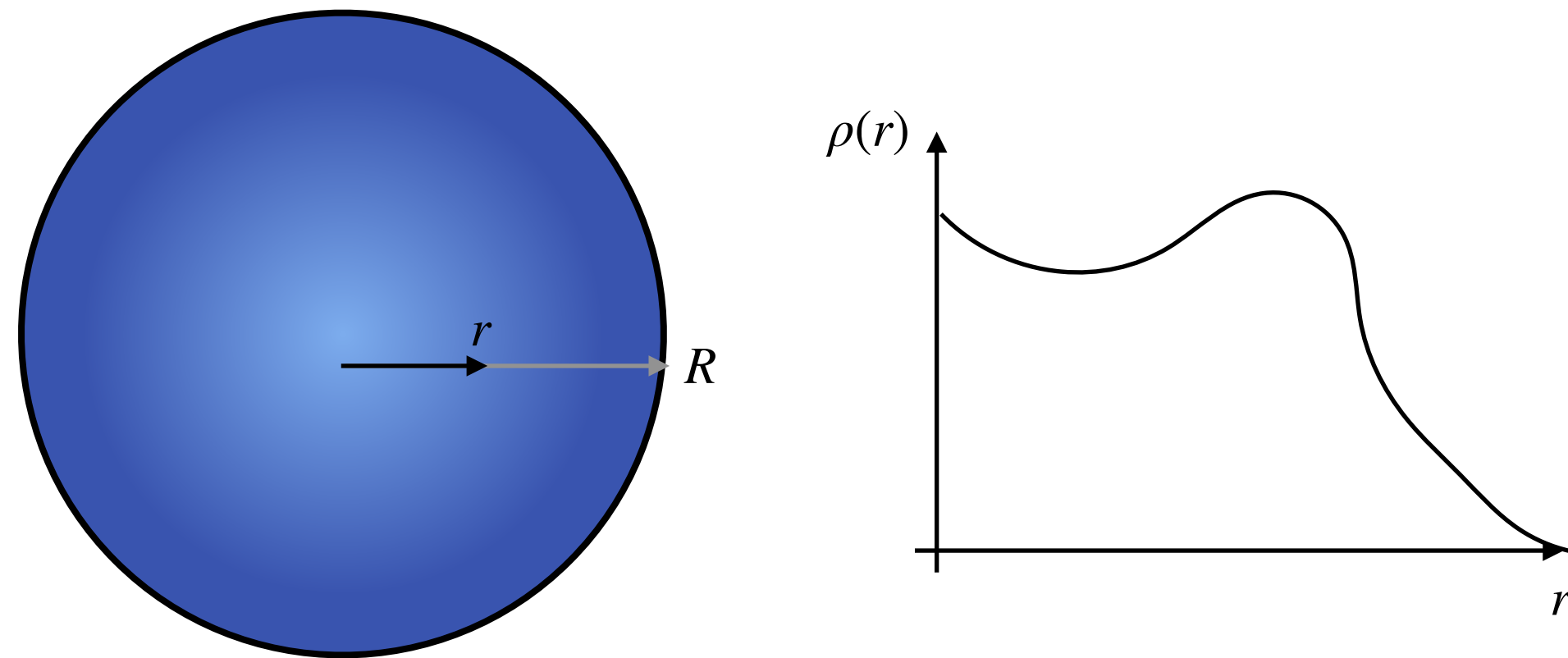
(A2) *If the outcome of measurement is the eigenvalue  $a_n$ , the system is left in the corresponding eigenstate  $\phi_n$  at the time just after measurement.*

The postulate (A1) is called the *statistical formula*, and (A2) the *measurement axiom*. The state change  $\psi \mapsto \phi_n$  described by the measurement axiom is called the *state reduction*.

You will understand this paragraph in the end of the course.

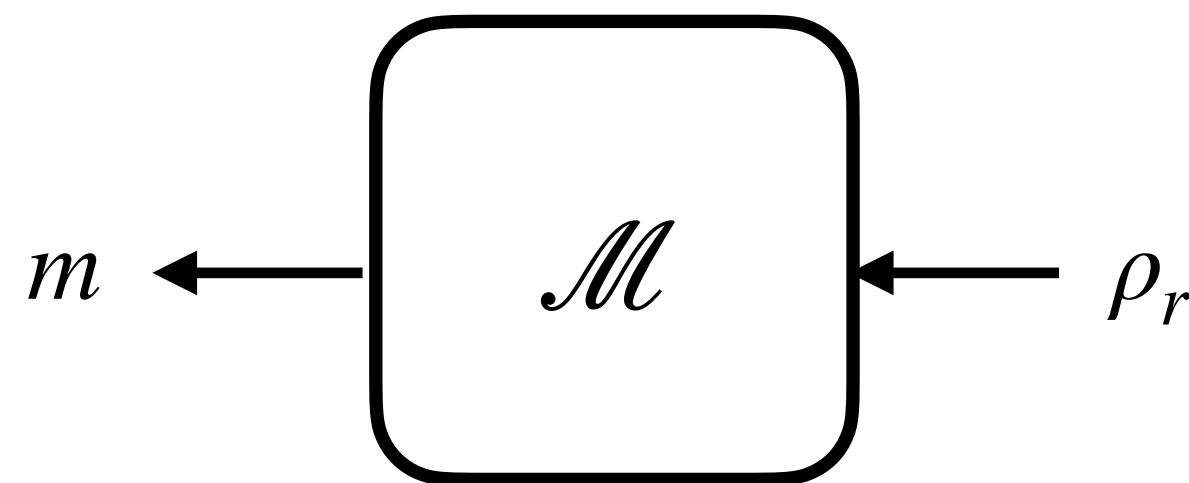
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## And Their Use in Physics



Density of a star/planet vs the radius from the center

Calculate total mass for a given density distribution



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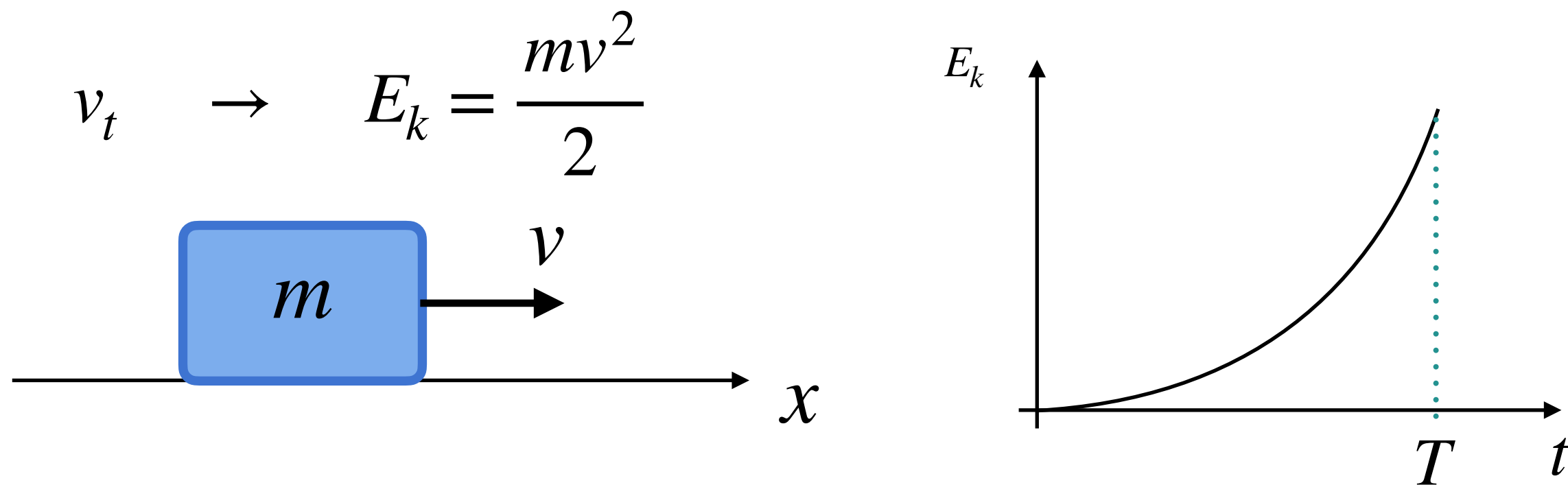
$\rho_r$

$m$



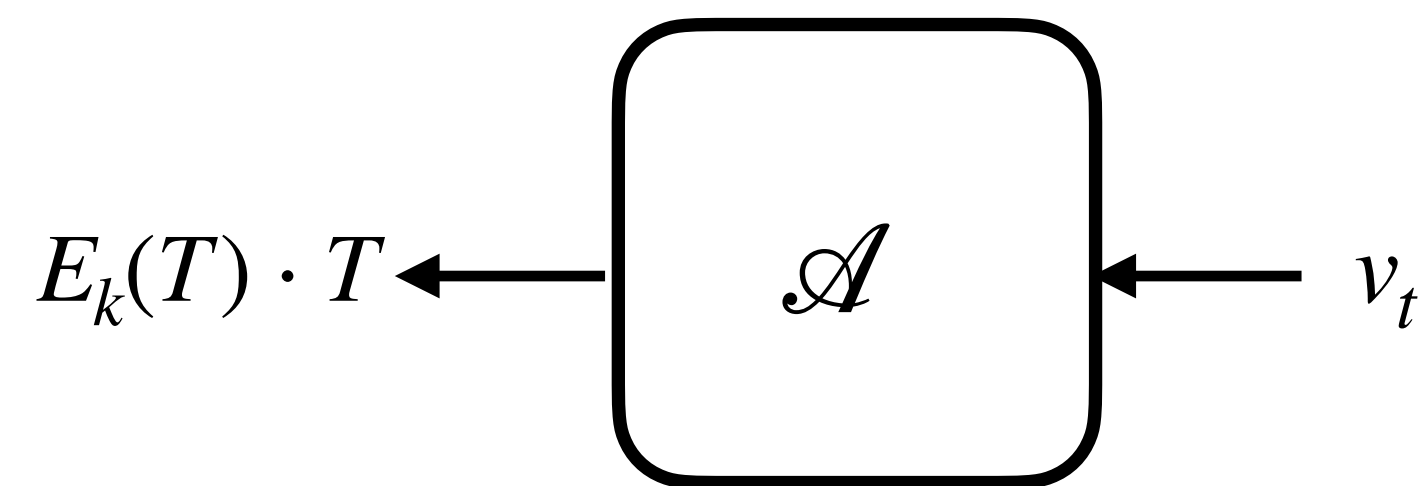
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## And Their Use in Physics



Calculate total “action” — energy\*time

Kinetic energy vs time



$\mathcal{A}$  : **function**  $\longrightarrow$  **number**

$v_t$                        $E_k(T) \cdot T$

Action  $A = Et$  is of fundamental importance.  
It is quantized, like electric charge  $q_e = e$

Exercise: Show that for constant acceleration,  $E_k t = px$