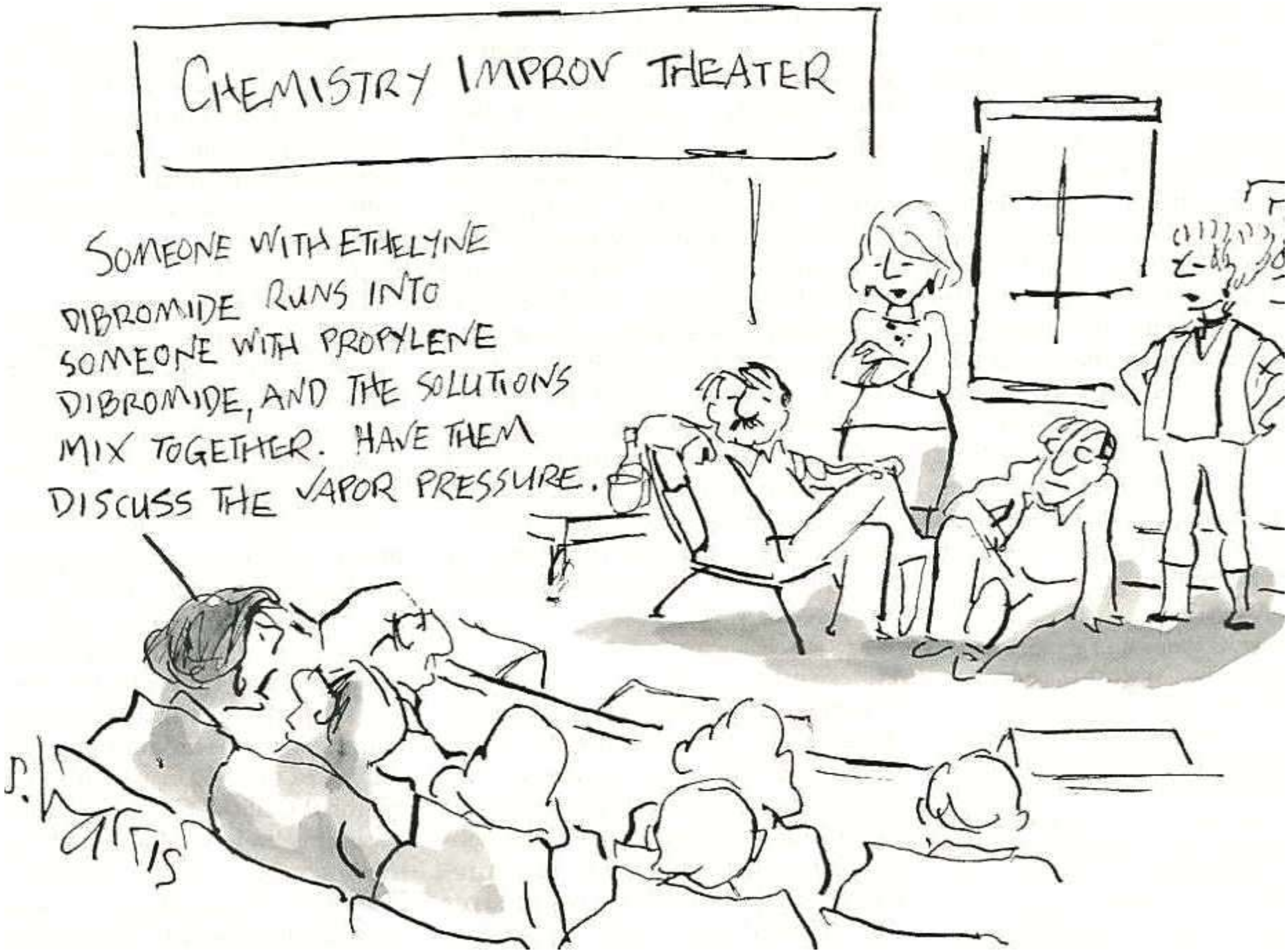

CHEMISTRY IMPROV THEATER
SOMEONE WITH ETHELYNE DIBROMIDE RUNS INTO SOMEONE WITH PROPYLENE DIBROMIDE, AND THE SOLUTIONS MIX TOGETHER. HAVE THEM DISCUSS THE VAPOR PRESSURE.
S. Harris

Canonical Equations of Motion -- Hamiltonian Dynamics

- From previous discussion: If the PE **U** is independent of velocities (conservative system) then the linear momentum in **rectangular coordinates** has the form: $\mathbf{p_i} = (\partial L/\partial \dot{\mathbf{x}}_i)$
- Extend this to the case where the Lagrangian is given in terms of generalized coordinates:

DEFINE: ***The Generalized Momentum*** (corresponding to the generalized coordinate $\mathbf{q_j}$): $\mathbf{p_j} \equiv (\partial L/\partial \dot{\mathbf{q}}_j)$.

$\mathbf{p_j} \equiv$ "Conjugate Momentum" to $\mathbf{q_j}$.

Or, "Canonically Conjugate Momentum"

- **(q,p) ≡ "conjugate" or "canonical" variables.**

- **Lagrange Eqtns of motion:** **s** degrees of freedom

$$(\partial L/\partial q_j) - (d/dt)[(\partial L/\partial \dot{q}_j)] = 0 \quad (j = 1,2,3, \ldots s)$$

- Gives **s** ***2nd order,*** time dependent, differential eqtns.

$\Rightarrow$ The system motion is determined for all time when **2s initial values** are specified: **s q_j's & s $\dot{q}_j$'s**

- We can represent the state of the system motion by the time dependent motion of a point in an abstract **s-dimensional configuration space** (coordinates = **s** generalized coords **q_j**).

- ***PHYSICS:*** In the **Lagrangian Formulation of Mechanics,** a system with **s** degrees of freedom = a problem in **s INDEPENDENT variables $q_j(t)$.** The generalized velocities, **$\dot{q}_j(t)$** are determined by taking the time derivatives of the **$q_j(t)$**. The velocities are not independent variables!

CONTRAST!

- **Hamiltonian Mechanics** is a ***fundamentally different*** picture!
- It describes the system motion in terms of ***1st order,*** time dependent equations of motion. The number of initial conditions is, of course, still **2s.**

$\Rightarrow$ We must describe the system motion with ***2s independent 1st order***, time dependent, differential equations expressed in terms of ***2s independent variables***.

- Choose **s** of these = **s generalized coordinates q_j.**
- The others = **s generalized (conjugate) momenta p_j.**

- **Hamiltonian Mechanics:**
- Describes the system motion in terms of **s generalized coordinates q_j & s generalized momenta p_j.** Gets **2s** ***1^{st} order,*** time dependent equations of motion.
- Recall again the ***DEFINITION:*** **Generalized Momentum** associated with generalized coord $\mathbf{q_j}$:

$$p_j \equiv (\partial L/\partial \dot{q}_j)$$

- **$(q,p) \equiv$ "conjugate" or "canonical" variables.**

Legendre Transformations

- ***Physically,*** the Lagrange formulation assumes the coordinates $\mathbf{q_j}$ are independent variables & the velocities $\dot{\mathbf{q}}_\mathbf{j}$ are dependent variables & are only obtained by taking time derivatives of the $\mathbf{q_j}$ once the problem is solved.
- ***Mathematically***, the Lagrange formalism treats $\mathbf{q_j}$ & $\dot{\mathbf{q}}_\mathbf{j}$ as independent variables. e.g., in Lagrange's eqtns, $(\partial L/\partial \mathbf{q_j})$ means take the partial derivative of L with respect to $\mathbf{q_j}$ keeping all other **q's** & ***ALSO*** all $\dot{\mathbf{q}}$**'s** constant. Similarly $(\partial L/\partial \dot{\mathbf{q}}_\mathbf{j})$ means take the partial derivative of L with respect to $\dot{\mathbf{q}}_\mathbf{j}$ keeping all other $\dot{\mathbf{q}}$**'s** & ***ALSO*** all **q's** constant.
- Treated as a pure mathematical problem, changing from the Lagrange formulation to the Hamilton formulation corresponds to changing variables from $(\mathbf{q},\dot{\mathbf{q}},\mathbf{t})$ ($\mathbf{q},\dot{\mathbf{q}}$, independent) to $(\mathbf{q},\mathbf{p},\mathbf{t})$ ($\mathbf{q},\mathbf{p}$ independent)

- **Lagrange's Equations** are:

$$(\partial L/\partial q_j) = (d/dt)[(\partial L/\partial \dot{q}_j)] \qquad (1)$$

- The **generalized momentum** is: $p_j = (\partial L/\partial \dot{q}_j)$ **(2)**
- **(1) & (2)** together $\Rightarrow$ $\dot{p}_j = (\partial L/\partial q_j)$ **(N's 2nd Law!!) (3)**
- From previous discussion, the ***Hamiltonian*** is:

$$H \equiv \sum_j \dot{q}_j (\partial L/\partial \dot{q}_j) - L \qquad (4)$$

- Rewrite **(4)** using the generalized momentum definition **(2)**:

$$\Rightarrow \quad H = \sum_j p_j \dot{q}_j - L \qquad (5)$$

- **(5)** is the starting point for **Hamiltonian Dynamics**.

Derivation of Hamilton's Equations

- **Lagrangian Dynamics:** Assumes the Lagrangian $\boldsymbol{L} = \boldsymbol{L}(\mathbf{q_j},\dot{\mathbf{q}}_j,\mathbf{t})$ (is a function of generalized coordinates, generalized velocities, and time).
- Solve each $\mathbf{p_j} = (\partial L/\partial \dot{\mathbf{q}}_j)$ for the generalized velocities & get: $\dot{\mathbf{q}}_j = \dot{\mathbf{q}}_j(\mathbf{q_k},\mathbf{p_k},\mathbf{t})$
- In the Hamiltonian $\mathbf{H} = \sum_j \mathbf{p_j} \dot{\mathbf{q}}_j - L$, make the change of variables from the set $(\mathbf{q_j},\dot{\mathbf{q}}_j,\mathbf{t})$ to the set $(\mathbf{q_k},\mathbf{p_k},\mathbf{t})$ & express the Hamiltonian as:

$$\mathbf{H} = \mathbf{H}(\mathbf{q_k},\mathbf{p_k},\mathbf{t}) = \sum_k \mathbf{p_k} \dot{\mathbf{q}}_k - L(\mathbf{q_k},\dot{\mathbf{q}}_k,\mathbf{t})$$

- **Hamiltonian Dynamics:** Always write

$$\mathbf{H = H(q_k,p_k,t) \quad = \sum_k p_k \dot{q}_k - \mathit{L}(q_k,\dot{q}_k,t)}$$

- This stresses that **Hamiltonian dynamics considers the generalized coordinates & generalized momenta as the variables:** $\mathbf{(q_k,p_k,t)}$**,** whereas **Lagrangian dynamics** considers the generalized coordinates & generalized velocities as the variables: $\mathbf{(q_k,\dot{q}_k,t)}$**.** A vital & important point!! Please keep it in mind!

- A proper **Hamiltonian** (for use in Hamiltonian dynamics) is ***ALWAYS*** ***(!)*** written as a function of the generalized coordinates & momenta: $\mathbf{H \equiv H(q_k,p_k,t)}$. **If you write it as a function of $\dot{q}_j$, it is NOT a Hamiltonian!!!**

- A proper **Lagrangian** (for use in Lagrangian dynamics) is ***ALWAYS*** ***(!)*** written as a function of the generalized coordinates & velocities: $\boldsymbol{L \equiv L(q_j,\dot{q}_j,t)}$

TO EMPHASIZE THIS

Consider a single free particle ($\vec{\mathbf{p}} = m\vec{\mathbf{v}}$)

Energy **= KE = T = (½)mv²** only. So, **H = T**

But, if it is a ***PROPER HAMILTONIAN***, can it be written $\mathbf{H = \frac{1}{2}mv^2}$?

NO!!!!!! **H** ***must*** be expressed in terms of the momentum **p**, not the velocity **v**! So the ***PROPER HAMILTONIAN*** is

$$\mathbf{H = [p^2/(2m)]} \qquad \textbf{!!!!!}$$

Derivation of Hamilton's Equations of Motion

- The Hamiltonian is: $\mathbf{H \equiv H(q_k,p_k,t)}$
- Take the total differential of **H**:

$$dH = \sum_k[(\partial H/\partial q_k)dq_k + (\partial H/\partial p_k)dp_k] + (\partial H/\partial t)dt \quad (1)$$

- Also:

$$H(q_k,p_k,t) = \sum_k p_k \dot{q}_k - L(q_k,\dot{q}_k,t) \qquad (2)$$

- The total differential of **(2)** is:

$$dH = \sum_k[\dot{q}_k\, dp_k + p_k\, d\dot{q}_k$$

$$- (\partial L/\partial q_k)dq_k - (\partial L/\partial \dot{q}_k)d\dot{q}_k] - (\partial L/\partial t)dt \qquad (3)$$

- We had: $\mathbf{p_k} = (\partial L/\partial \dot{\mathbf{q}}_k)$ and $\dot{\mathbf{p}}_k = (\partial L/\partial \mathbf{q}_k)$
- Put these into **(3)** & get**:**

$$\mathbf{dH = \sum_k[\dot{q}_k\, dp_k + p_k\, d\dot{q}_k - p_k\, d\dot{q}_k - \dot{p}_k\, dq_k] - (\partial L/\partial t)dt}$$

Or:

$$\mathbf{dH = \sum_k [\dot{q}_k\, dp_k - \dot{p}_k\, dq_k\,] - (\partial L/\partial t)dt} \qquad \mathbf{(4)}$$

- Compare **(4)** with **(1)** **& get:**

$$\mathbf{\dot{q}_k = (\partial H/\partial p_k), \quad \dot{p}_k = - (\partial H/\partial q_k)}$$

$$\mathbf{(\partial H/\partial t) = - (\partial L/\partial t)}$$

Hamilton's Equations of Motion

$$\dot{q}_k = (\partial H/\partial p_k) \qquad \dot{p}_k = -(\partial H/\partial q_k)$$

- We also have: $(\partial H/\partial t) = -(\partial L/\partial t)$
- Use **Hamilton's Equations** in **(1):**

$$dH = \sum_k[(\partial H/\partial q_k)dq_k + (\partial H/\partial p_k)dp_k] + (\partial H/\partial t)dt \quad (1)$$

- From Hamilton's Equations, each term in the sum = 0 & **(1)** becomes: $(dH/dt) = (\partial H/\partial t)$ **(5)**
- **(5)** $\Rightarrow$ If there is no ***explicit*** time dependence in **H**, $(\partial H/\partial t) = 0$, then total time derivative $(dH/dt) = 0$ or **H = constant in time**. (**H is conserved**.) If conditions are such that **H = E** (total energy), then the total energy is conserved!

- ***Hamilton's Equations of Motion***

$$\dot{q}_k = (\partial H/\partial p_k) \qquad \dot{p}_k = -(\partial H/\partial q_k)$$

- These are called **the "canonical" equations of motion** because of their (almost) symmetric appearance.
- The description of motion based on these is called **Hamiltonian Dynamics.**

- ***Hamilton's Equations of Motion***

$$\dot{q}_k = (\partial H/\partial p_k) \qquad \dot{p}_k = -(\partial H/\partial q_k)$$

- Consider a system with **3n** coordinates, **m** constraints & **s = 3n - m** degrees of freedom.

  ⇒ **Lagrangian Dynamics** description is in terms of **s** Lagrange's Eqtns of Motion (2nd order differential eqtns).

  ⇒ **Hamiltonian Dynamics** description is in terms of **2s** Hamilton's Eqtns of Motion (1st order differential eqtns).

- Since one can be derived from the other, obviously, the 2 descriptions are **100% equivalent**. They are also 100% equivalent to Newton's 2nd Law!

Discussion of Hamilton's Eqtns

- **Hamiltonian: $H(q,p,t) = \sum_k \dot{q}_k p_k - L(q,\dot{q},t)$** **(a)**

  Hamilton's Equations of Motion:

$\dot{q}_k = (\partial H/\partial p_k)$ **(b)**, $\dot{p}_k = -(\partial H/\partial q_k)$ **(c)**, $-(\partial L/\partial t) = (\partial H/\partial t)$ **(d)**

- **2n** ***1st order***, time dependent equations of motion **replacing** the **n 2nd order** Lagrange Equations of motion.
- **(a):** The formal definition of the Hamiltonian **H** in terms of the Lagrangian ***L***. However, as we'll see, in practice, we often needn't know ***L*** first to be able to construct **H**.
- **(b): $\dot{q}_k = (\partial H/\partial p_k)$:** Gives **$\dot{q}_k$'s** as functions of **(q,p,t).**

  $\Rightarrow$ Given initial values, integrate to get $q_k = q_k(q,p,t) \Rightarrow$ Form the "inverse" of relns of the eqtns $p_k = (\partial L/\partial \dot{q}_k)$ which give $p_k = p_k(q,\dot{q},t)$. $\Rightarrow$ "No new information".

- **Hamiltonian**: **$H(q,p,t) = \sum_k \dot{q}_k p_k - L(q,\dot{q},t)$** **(a)**

Hamilton's Equations of Motion:

$\dot{q}_k = (\partial H/\partial p_k)$ **(b)**, $\dot{p}_k = -(\partial H/\partial q_k)$ **(c)**, $-(\partial L/\partial t) = (\partial H/\partial t)$ **(d)**

- **(b): $\dot{q}_k = (\partial H/\partial p_k)$: $\Rightarrow$ $\dot{q}_k = \dot{q}_k(q,p,t)$. $\Rightarrow$** "No new info".
  - Usually true in terms of **SOLVING** mechanics problems. However, within the Hamiltonian picture of mechanics, where **$H = H(q,p,t)$,** obtained **NO MATTER HOW** (not necessarily by **(a)**), this has equal footing (& contains equally important information as **(c)**).
- **(c): $\dot{p}_k = -(\partial H/\partial q_k)$:** Integrate & get **$p_k = p_k(q,p,t)$**
- **(d): $-(\partial L/\partial t) = (\partial H/\partial t)$:** This is obviously only important in time dependent problems.

Recipe for Hamiltonian Mechanics

- **Hamiltonian:** $H(q,p,t) = \sum_k \dot{q}_k p_k - L(q,\dot{q},t)$ **(a)**

  Hamilton's Equations of Motion:

  $\dot{q}_i = (\partial H/\partial p_i)$ **(b)**, $\dot{p}_i = -(\partial H/\partial q_i)$ **(c)**, $-(\partial L/\partial t)=(\partial H/\partial t)$ **(d)**

- **Recipe:**

  1. Set up the Lagrangian, $L = T - U = L(q,\dot{q},t)$

  2. Compute **s** conjugate momenta using: $p_k \equiv (\partial L/\partial \dot{q}_k)$

  3. Form the Hamiltonian **H** from **(a).**

  This will be of the "mixed" form $H = H(q,\dot{q},p,t)$

  4. Invert **s** $p_k \equiv (\partial L/\partial \dot{q}_k)$ to get $\dot{q}_k \equiv \dot{q}_k(q,p,t)$.

  5. Apply the results of **4**. to eliminate $\dot{q}_k$ from **H** to get a

  proper Hamiltonian $H = H(q,p,t)$.

Then & only then can you properly & correctly use **(b)** & **(c)** to get the equations of motion!

- If you think that this is a long, tedious process, you aren't alone!
  - This requires that you set up the Lagrangian first!
  - If you already have the Lagrangian, why not go ahead & do Lagrangian dynamics instead of going through all of this to do Hamiltonian dynamics?
  - Further, combining the **2s** 1st order differential equations of motion

$$\dot{q}_k = (\partial H/\partial p_k) \quad (b) \quad \& \quad \dot{p}_k = -(\partial H/\partial q_k) \quad (c)$$

gives the **SAME** **s** 2nd order differential equations of motion that Lagrangian dynamics gives!

- However, fortunately, for many physical systems of interest, it's possible to considerably shorten this procedure, even eliminating many steps completely!

Hamiltonian Dynamics Recipe (Comments)

1. In simple cases, its often possible to directly set up **H** in terms of generalized coordinates & momenta: $\mathbf{H(q_k,p_k,t)}$. This is because the identification of the generalized momenta $\mathbf{p_k}$ is easy.

2. Unfortunately, in more complicated cases, where identification of the $\mathbf{p_k}$ is more difficult, it actually might be necessary to first set up the Lagrangian ***L***, & then calculate $\mathbf{p_k}$ with $\mathbf{p_k = (\partial \mathit{L}/\partial \dot{q}_k)}$

3. ***Only after you have*** $\mathbf{H = H(q_k,p_k,t)}$ can you apply Hamilton's Eqtns! $\mathbf{\dot{q}_k = (\partial H/\partial p_k)}$, $\mathbf{\dot{p}_k = -(\partial H/\partial q_k)}$

- ***In many cases***, we know that

$$\Rightarrow \mathbf{H = T + U}$$

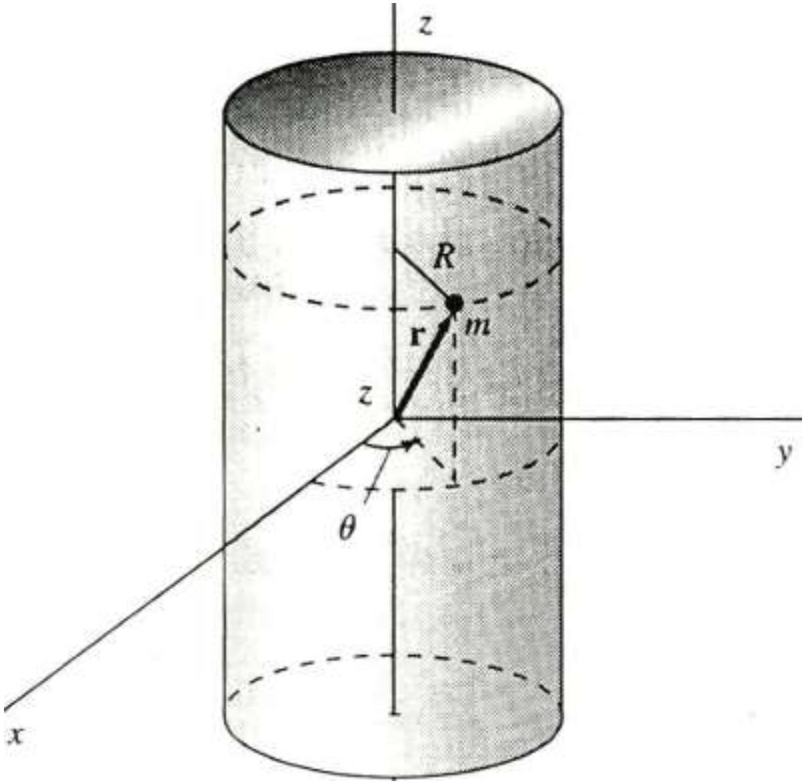
That is, in many cases, the Hamiltonian is automatically the total mechanical energy E

- If that is the case, we can ***skip many steps*** of the recipe. Instead: **1)** Write **H = T + U** ***immediately.*** Express **T** in terms of the **MOMENTA** $\mathbf{p_k}$ (**not** the velocities $\dot{\mathbf{q}}_\mathbf{k}$). Often it's easy to see how the $\mathbf{p_k}$ depend on the $\dot{\mathbf{q}}_\mathbf{k}$ & thus its easy to do this. Once this is done, we can **go ahead & do Hamiltonian Dynamics** without ever having written the Lagrangian.

Example 7.11

- Use the Hamiltonian method to find the equations of motion of a particle of mass **m**, constrained to move on the surface of a cylinder defined by $\mathbf{x^2 + y^2 = R^2}$. The particle is subject to a force directed towards the origin and proportional to the distance of the particle from the origin:

  $\vec{\mathbf{F}} = -\mathbf{k}\vec{\mathbf{r}}$. Worked on the board!



Comments

- We could have done this problem with **Lagrangian** mechanics! In fact, in this case, **Lagrange's Equations** are easier to get than **Hamilton's Equations.**
- **This is often true!** The **Lagrangian Method** often leads more easily to the equations of motion than the **Hamiltonian Method.** (In my opinion, almost always!)
- In the **Hamiltonian method,** $\mathbf{q_k}$ & $\mathbf{p_k}$ are considered independent. In the **Lagrangian Method** $\mathbf{q_k}$, $\dot{\mathbf{q}}_\mathbf{k}$ are not.

  $\Rightarrow$ **The Hamiltonian Method** sometimes has a practical advantage over the **Lagrangian Method.**
  - e. g., Useful in celestial mechanics: Looking at motions of bodies due to perturbations of other bodies.
- In general, main power of **Hamiltonian** formulation is its use as a basis for sub-areas of physics beyond classical mechanics.
  - Quantum mechanics and beyond!