Connecting Dots

From Hamilton's Principle to Schrödinger's Equation

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Nature is just as lazy as us

Introduction

Lagrangian:

$$\mathcal{L}(q_1, q_2, \ \ldots\ , q_n, \dot{q_1}, \dot{q_2}, \ \ldots\ , \dot{q_n}, t) = \mathcal{L}(q, \dot{q}, t) = T - U$$

Action:

$$S = \int_{t_1}^{t_2} \mathcal{L} \text{ dt}$$

Hamilton's Principle

Hamilton's Principle: The system's physical path is the one for which the action S is minimal.

$$\delta S = 0$$

$$\frac{\partial \mathcal{L}}{\partial q_i} - \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) = 0$$

Apparently, we care about invariance

Change of coordinates (q $\rightarrow Q$) :

$$Q_k = Q_k(q, t)$$

$$q_k = q_k(Q, t)$$

$$\dot{q_k} = \sum_i \left(\frac{\partial q_k}{\partial Q_i} \dot{Q}_i \right) + \frac{\partial q_k}{\partial t}$$

And so, we have:

$$\dot{q_k} = \dot{q_k}(Q, \dot{Q}, t)$$

Apparently, we care about invariance

Transformed Lagrangian:

$$\bar{\mathcal{L}}(Q, \dot{Q}, t) = \mathcal{L}(q(Q, t), \dot{q}(Q, \dot{Q}, t), t)$$

$$\frac{\partial \bar{\mathcal{L}}}{\partial \dot{Q}_i} = \sum_k \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \frac{\partial q_k}{\partial Q_i}$$

$$\frac{d}{dt}\left(\frac{\partial \bar{\mathcal{L}}}{\partial \dot{Q}_i}\right) = \sum_k \left(\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k}\right) \frac{\partial q_k}{\partial Q_i} + \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \frac{\partial \dot{q}_k}{\partial Q_i}\right)$$

Apparently, we care about invariance

$$\frac{\partial \bar{\mathcal{L}}}{\partial Q_i} = \sum_k \left(\frac{\partial \mathcal{L}}{\partial q_k} \frac{\partial q_k}{\partial Q_I} + \frac{\partial \mathcal{L}}{\partial \dot{q}_k} \frac{\partial \dot{q}_k}{\partial Q_i} \right)$$

$$\frac{d}{dt} \left(\frac{\partial \bar{\mathcal{L}}}{\partial \dot{Q}_i} \right) - \frac{\partial \bar{\mathcal{L}}}{\partial Q_i} = \sum_k \left(\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k} \right) - \frac{\partial \mathcal{L}}{\partial q_k} \right) \frac{\partial q_k}{\partial Q_i} = 0$$

Getting less lazy

Legendre done wrong

The conjugate momentum:

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q}_k}$$

The hamiltonian:

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

It is the energy... kinda?

Legendre done wrong

Hamilton's equations:

$$\dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} \qquad \dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i}$$

There's a third one, which we won't really care about:

$$\frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}$$

Legendre done wrong

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Variational methods strike back

$$\mathcal{L} = \sum_k p_k \dot{q}_k - H$$

We can write the action as:

$$S = \int_{t1}^{t2} \sum_k p_k \dot{q}_k - H \ \mathrm{dt}$$

This gives us Hamilton's equations

Invariance is on steroids now

Canonical transformations

Change of coordinates in phase space $(q, p) \to (Q, P)$:

$$Q_k = Q_k(q, p, t) \quad P_k = P_k(q, p, t)$$

$$\dot{Q}_i = \frac{\partial \mathcal{K}}{\partial P_i} \quad \dot{P}_i = -\frac{\partial \mathcal{K}}{\partial Q_i}$$

$\mathcal{K}(Q, P, t)$ is the transformed Hamiltonian.

Canonical transformations

$$\sum_k (P_k dQ_k - p_k dq_k) + (\mathcal{K} - \mathcal{H})dt = d\Phi$$

If this equation is satisfied, we have a canonical transformation.

Generating Functions

Natural choice is $\Phi = F(q, Q, t)$

$$p_i = \frac{\partial F}{\partial q_i} \quad P_i = \frac{\partial F}{\partial Q_i}$$

Transformed Hamiltonian is:

$$\mathcal{K}(Q, P, t) = \mathcal{H}(Q, P, t) + \frac{\partial F}{\partial t}$$

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More generating functions

New generating function:

$$G(q,P,t) = \sum_i P_i Q_i + F(q, Q(q,P,t), t)$$

Skipping a few steps:

$$p_i = \frac{\partial G}{\partial q_i} \quad Q_i = \frac{\partial G}{\partial P_i}$$

And the transformed Hamiltonian is:

$$\mathcal{K} = \mathcal{H} + \frac{\partial G}{\partial t}$$

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Sympletic approach

$$Q_i = Q_i(q,p) \quad P_i = P_i(q,p)$$

$$\dot{Q}_i = \sum_k \frac{\partial Q_i}{\partial q_k}\dot{q}_k + \frac{\partial Q_i}{\partial p_k}\dot{p}_k$$

$$\dot{Q}_i = \sum_k \frac{\partial Q_i}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial Q_i}{\partial p_k}\frac{\partial H}{\partial q_k}$$

Sympletic approach

$$Q_i = Q_i(q,p) \quad P_i = P_i(q,p)$$

$$\dot{Q}_i = \sum_k \frac{\partial Q_i}{\partial q_k}\dot{q_k} + \frac{\partial Q_i}{\partial p_k}\dot{p_k}$$

$$\dot{Q}_i = \sum_k \frac{\partial Q_i}{\partial q_k}\frac{\partial H}{\partial p_k} - \frac{\partial Q_i}{\partial p_k}\frac{\partial H}{\partial q_k}$$

Sympletic approach

Inverse:

$$q_k = q_k(Q,P) \quad p_k = p_k(Q,P)$$

Then:

$$\frac{\partial \mathcal{H}}{\partial P_i} = \sum_k \frac{\partial \mathcal{H}}{\partial q_k}\frac{\partial q_k}{\partial P_i} + \frac{\partial \mathcal{H}}{\partial p_k}\frac{\partial p_k}{\partial P_i}$$

Sympletic approach

Inverse:

$$q_k = q_k(Q, P) \quad p_k = p_k(Q, P)$$

Then:

$$\frac{\partial \mathcal{H}}{\partial P_i} = \sum_k \frac{\partial \mathcal{H}}{\partial q_k}\frac{\partial q_k}{\partial P_i} + \frac{\partial \mathcal{H}}{\partial p_k}\frac{\partial p_k}{\partial P_i}$$

Sympletic Approach

$$\dot{Q}_i = \frac{\partial \mathcal{H}}{\partial P_i}$$

if:

$$\left(\frac{\partial Q_i}{\partial q_k}\right)_{(q,p)} = \left(\frac{\partial q_k}{\partial P_i}\right)_{(Q,P)} \quad \left(\frac{\partial Q_i}{\partial p_k}\right)_{(q,p)} = -\left(\frac{\partial p_k}{\partial P_i}\right)_{(Q,P)}$$

Sympletic Approach

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if:

$$\left(\frac{\partial Q_i}{\partial q_k}\right)_{(q,p)} = \left(\frac{\partial q_k}{\partial P_i}\right)_{(Q,P)} \quad \left(\frac{\partial Q_i}{\partial p_k}\right)_{(q,p)} = -\left(\frac{\partial p_k}{\partial P_i}\right)_{(Q,P)}$$

All over again

Same procedure with $\dot{P}_i$ and $\frac{\partial \mathcal{H}}{\partial Q_i}$:

$$\left(\frac{\partial P_i}{\partial q_k}\right)_{(q,p)} = -\left(\frac{\partial p_k}{\partial Q_i}\right)_{(Q,P)} \quad \left(\frac{\partial P_i}{\partial p_k}\right)_{(q,p)} = \left(\frac{\partial q_k}{\partial Q_i}\right)_{(Q,P)}$$

$$\mathcal{K}(Q,P,t) = \mathcal{H}(q(Q,P), p(Q,P), t)$$

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We love matrices

$$\hat{\eta} = \begin{pmatrix} q_1 \\ q_2 \\ \vdots \\ q_n \\ p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix} \quad \hat{\zeta}(\hat{\eta}) = \begin{pmatrix} Q_1(q,p) \\ Q_2(q,p) \\ \vdots \\ Q_n(q,p) \\ P_1(q,p) \\ P_2(q,p) \\ \vdots \\ P_n(q,p) \end{pmatrix}$$

We love matrices

$$\frac{\partial \mathcal{H}}{\partial \hat{\eta}} = \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial q_1} \\ \vdots \\ \frac{\partial \mathcal{H}}{\partial q_n} \\ \frac{\partial \mathcal{H}}{\partial p_1} \\ \vdots \\ \frac{\partial \mathcal{H}}{\partial p_n} \end{pmatrix} \quad \frac{\partial \mathcal{H}}{\partial \hat{\zeta}} = \begin{pmatrix} \frac{\partial \mathcal{H}}{\partial Q_1} \\ \vdots \\ \frac{\partial \mathcal{H}}{\partial Q_n} \\ \frac{\partial \mathcal{H}}{\partial P_1} \\ \vdots \\ \frac{\partial \mathcal{H}}{\partial P_n} \end{pmatrix}$$

We love matrices

$$\hat{J} = \begin{pmatrix} \mathcal{O}_n & \mathcal{I}_n \\ -\mathcal{I}_n & \mathcal{O}_n \end{pmatrix}$$

$$\hat{J}^2 = -\mathcal{I}_{2n}$$

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

$$\det \hat{J} = 1$$

We love matrices

Hamilton's equations for (q, p) and (Q, P):

$$\dot{\hat{\eta}} = \hat{J}\frac{\partial \mathcal{H}}{\partial \hat{\eta}} \quad \dot{\hat{\zeta}} = \hat{J}\frac{\partial \mathcal{H}}{\partial \hat{\zeta}}$$

$$\dot{\hat{\zeta}} = \hat{M}\dot{\hat{\eta}} \qquad \frac{\partial \mathcal{H}}{\partial \hat{\eta}} = \hat{M}^T\frac{\partial \mathcal{H}}{\partial \hat{\zeta}}$$

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I promise this simplifies things

Then:

$$\hat{J}\frac{\partial \mathcal{H}}{\partial \hat{\zeta}} = \hat{M}\hat{J}\hat{M}^T\frac{\partial \mathcal{H}}{\partial \hat{\zeta}}$$

$$\hat{M}\hat{J}\hat{M}^T = \hat{M}^T\hat{J}\hat{M} = \hat{J}$$

Canonical transformation jacobian matrices are part of the sympletic group $Sp_{(2n,\mathbb{R})}$

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Canonical transformation jacobian matrices are part of the sympletic group $Sp_{(2n,\mathbb{R})}$

Poisson Brackets

$$F(q, \dot{q}, t):$$

$$\frac{dF}{dt} = \sum_k \frac{\partial F}{\partial q_k}\frac{\partial \mathcal{H}}{\partial p_k} - \frac{\partial F}{p_k}\frac{\partial \mathcal{H}}{\partial q_k} + \frac{\partial F}{\partial t}$$

$$\frac{dF}{dt} = \{F, H\} + \frac{\partial F}{\partial t}$$

$$\{F, G\} = \sum_k \frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k} - \frac{\partial F}{p_k}\frac{\partial G}{\partial q_k}$$

Canonical invariants

$$\{F, G\}_{\hat{\eta}} = \left(\frac{\partial F}{\partial \hat{\eta}}\right)^T \hat{J} \frac{\partial G}{\partial \hat{\eta}}$$

$$\{F, G\}_{\hat{\eta}} = \left(\hat{M}^T \frac{\partial F}{\partial \hat{\zeta}}\right)^T \hat{J} \left(\hat{M}^T \frac{\partial G}{\partial \hat{\zeta}}\right)$$

Canonical invariants

$$\{F,G\}_{\hat{\eta}} = \left(\frac{\partial F}{\partial \hat{\zeta}}\right)^T \hat{M}\hat{J}\hat{M}^T \frac{\partial G}{\partial \hat{\zeta}}$$

$$\{F,G\}_{\hat{\eta}} = \{F,G\}_{\hat{\zeta}}$$

Poisson brackets are canonical invariants!

Poisson brackets and Quantum Theory

Properties:

$$\{A, B\} = -\{B, A\}$$
$$\{A + \alpha B, C\} = \{A, C\} + \alpha\{B, C\}$$
$$\{AB, C\} = A\{B, C\} + \{A, C\}B$$
$$\{\{A, B\}, C\} + \{\{B, C\}, A\} + \{\{C, A\}, B\} = 0$$

Poisson brackets and Quantum Theory

Generates a Lie Algebra!

What else generates a Lie Algebra? Cross product and matrix commutator!

Similarities between theories: Heisenberg's representation and Poisson Brackets formulation:

$$\frac{1}{i\hbar}[\hat{A},\hat{B}] \xrightarrow{\hbar\longrightarrow 0} \{A,B\}$$

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Action as a generator

Infinitesimal transformations

$$Q_i = q_i + \delta q_i = q_i + \epsilon f_i(q,p,t) \quad P_i = p_i + \delta p_i = p_i + \epsilon g_i(q,p,t)$$

Remember:

$$\sum_i p_i dq_i - P_i dQ_i = d\Phi$$

Using $\Phi = \epsilon F$:

$$\sum_i g_i dq_i + p_i df_i = -dF$$

Infinitesimal transformations

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Remember:

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Using $\Phi = \epsilon F$:

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Infinitesimal transformations

$$G = \sum_i p_i f_i + F:$$

$$\sum_i g_i dq_i - f_i dp_i = -dG$$

$$\delta\hat{\eta} = \epsilon\{\hat{\eta}, G\}$$

Time evolution

$$\epsilon = \mathsf{dt} \quad G = \mathcal{H}$$

$$\delta q_i = \dot{q}_i \mathsf{dt} \quad \delta p_i = \dot{p}_i \mathsf{dt}$$

$$Q_i = q_i(t + \mathsf{dt}) \quad P_i = p_i(t + \mathsf{dt})$$

Time evolution

$t \to t + dt$:

$$\Phi = \epsilon F = \mathsf{dt}(H - \sum_i p_i \dot{q}_i) = -\mathcal{L}\ \mathsf{dt}$$

$t_0 \to t$:

$$\Phi = -\int_{t_0}^{t} \mathcal{L}\ \mathsf{dt} = -S$$

$t \to t_0$:

$$\Phi = S$$

Time evolution

$t \to t + dt$:

$$\Phi = \epsilon F = \mathsf{dt}(H - \sum_i p_i \dot{q}_i) = -\mathcal{L}\ \mathsf{dt}$$

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Time evolution

$t \to t + dt$:

$$\Phi = \epsilon F = \mathsf{dt}(H - \sum_i p_i \dot{q}_i) = -\mathcal{L}\ \mathsf{dt}$$

$t_0 \to t$:

$$\Phi = -\int_{t_0}^{t} \mathcal{L}\ \mathsf{dt} = -S$$

$t \to t_0$:

$$\Phi = S$$

Almost There

Hamilton-Jacobi Equation

Generating function $F(q, P, t)$:

$$p_i = \frac{\partial F}{\partial q_i} \quad Q_i = \frac{\partial F}{\partial P_i}$$

$$\mathcal{H} + \frac{\partial F}{\partial t} = \mathcal{K}$$

Hamilton-Jacobi Equation

$$\mathcal{K} = 0$$

$$Q_i = \beta_i \quad P_i = \alpha_i$$

$$\mathcal{H}(q, p, t) + \frac{\partial F}{\partial t} = 0$$

$$p_i = \frac{\partial F}{\partial q_i} \quad \beta_i = \frac{\partial F}{\partial \alpha_i}$$

Hamilton-Jacobi Equation

$$F = S(q, \alpha, t)$$

Hamilton-Jacobi Equation:

$$\mathcal{H}(q, \frac{\partial S}{\partial q}, t) + \frac{\partial S}{\partial t} = 0$$

Hamilton-Jacobi Equation

$$\frac{dS}{dt} = \sum_i \frac{\partial S}{\partial q_i}\dot{q}_i + \frac{\partial S}{\partial t}$$

$$\frac{dS}{dt} = \sum_i p_i \dot{q}_i - \mathcal{H} = \mathcal{L}$$

$$S = \int \mathcal{L}\ \mathrm{dt} + \mathrm{constant}$$

Separation of variables

$\mathcal{H}$ independent of time:

$$S = W(q) - \alpha_1 t$$

$$\alpha_1 = \mathcal{H}$$

$$\frac{\partial S}{\partial q_i} = \frac{\partial W}{\partial q_i} = p_i$$

Separation of variables

$\mathcal{H}$ independent of q_i:

$$S = W_1(q_1, \ \dots \ , q_{i-1}, q_{i+1}, \ \dots \ , q_n, t) + \alpha_i q_i$$

Grand Finale

Geometric Optics

$$\frac{1}{2m}\left(\left(\frac{\partial S}{\partial x}\right)^2+\left(\frac{\partial S}{\partial y}\right)^2+\left(\frac{\partial S}{\partial z}\right)^2\right)+V(x,y,z)+\frac{\partial S}{\partial t}=0$$

$$\frac{1}{2m}|\nabla S|^2+V(x,y,z)+\frac{\partial S}{\partial t}=0$$

$$S(x,y,z,t)=W(x,y,z)-Et$$

Geometric Optics

$$\vec{p} = \nabla W \text{ and } |\nabla W| = \sqrt{2m(E - V)}$$

$$S = \text{Phase}$$

Geometric Optics

Two surfaces $S = C$:

$$\frac{dW}{dt} - E = 0$$

$$E = |\nabla W| \frac{dl}{dt}$$

$$\frac{dl}{dt} = v = \frac{E}{\sqrt{2m(E-V)}}$$

Geometric Optics

Phase velocity $\neq$ particle's velocity!

$$v_g = \frac{d\omega}{dt}$$

$$p = \hbar k \quad E = 2\pi\hbar\nu$$

$$\omega = \frac{V}{\hbar} + \frac{\hbar k^2}{2m}$$

Geometric Optics

$$v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m}$$

$$v_g = \frac{p}{m}$$

Schrödinger's Equation

Schrödinger conjectured:

$$\Psi = \exp\left\{\frac{iS}{\hbar}\right\}$$

$$S = -i\hbar \ln \Psi$$

$$\frac{\partial S}{\partial x} = \frac{-i\hbar}{\Psi}\frac{\partial \Psi}{\partial x}$$

Schrödinger's Equation

$$\frac{-\hbar^2}{2m\Psi^2}|\nabla\Psi|^2 + V = \frac{i\hbar}{\Psi}\frac{\partial\Psi}{\partial t}$$

Wrong??

Schrödinger's Equation

$$\frac{\partial^2 S}{\partial x^2} = \frac{i\hbar}{\Psi^2}\left(\frac{\partial \Psi}{\partial x}\right)^2 - \frac{i\hbar}{\Psi}\frac{\partial^2 \Psi}{\partial x^2}$$

$$\frac{\partial^2 S}{\partial x^2} = \frac{\partial p_x}{\partial x} = \frac{\partial^2 \mathcal{L}}{\partial x \partial \dot{x}}$$

$$\mathcal{L} = \frac{m(\dot{x}^2 + \dot{y}^2 + \dot{z}^2)}{2} - V(x, y, z)$$

Schrödinger's Equation

$$\frac{\partial^2 S}{\partial x^2} = 0$$

$$\frac{1}{\Psi}\left(\frac{\partial \Psi}{\partial x}\right)^2 = \frac{\partial^2 \Psi}{\partial x^2}$$

$$\frac{1}{\Psi}|\nabla \Psi|^2 = \nabla^2 \Psi$$

Schrödinger's Equation

$$\frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

Using $S(x, y, z, t) = W(x, y, z) - Et$:

$$\frac{-\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi$$