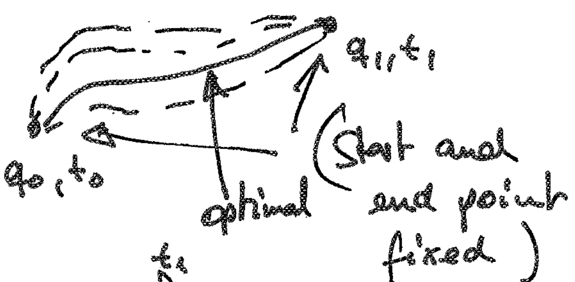
4. Canonical Formalism

4.1. Hamilton–Jacobi Theory

Consider the action S as a function of the coordinates $q = (q_1, \dots, q_N)$ and time t of the end point

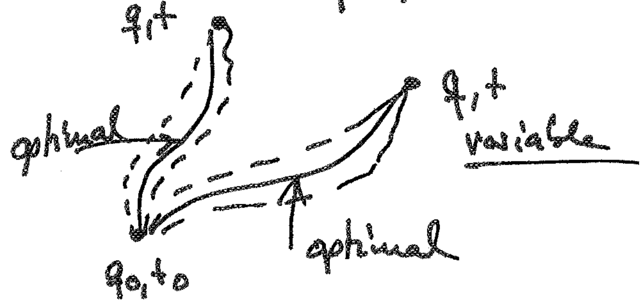
Principle of least action



$$S = \int_{t_0}^{t_1} L(q(t), \dot{q}(t), t)\, dt$$

$$q(t_0) = q_0 \ , \ q(t_1) = q_1$$

Action $S(q,t)$



each trajectory with minimal S

$$S(q,t) = \int_{t_0}^{t} dt' \, L(q(t'), \dot{q}(t'), t')$$

$$q(t_0) = q_0$$

- Consider infinitesimal shift of the end q:

$$\delta S = \frac{\partial S}{\partial q} \delta q(t)$$

$$\delta q(t_0) = 0$$

we can also write

$$\delta S = \int_{t_0}^{t} dt' \left(\frac{\partial L}{\partial q} \delta q(t') + \frac{\partial L}{\partial \dot{q}} \delta \dot{q}(t') \right)$$

$$\underset{\substack{\text{integrate} \\ \text{by parts}}}{=} \int_{t_0}^{t} dt' \underbrace{\left(\frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} \right)}_{\substack{=0 \text{ since we choose} \\ \text{only optimal trajectories}}} \delta q(t') + \frac{\partial L}{\partial \dot{q}} \delta q(t') \Big|_{t_0}^{t}$$

$$= \frac{\partial L}{\partial \dot{q}} \delta q(t)$$

$$\Rightarrow \boxed{\frac{\partial S}{\partial q} = p \quad , \quad p = \frac{\partial L}{\partial \dot{q}} \quad \text{canonical momentum}}$$

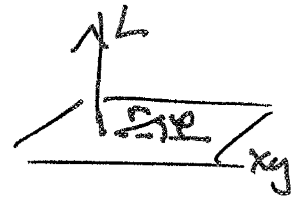
<u>Examples</u>: Canonical momentum

a) $L = \frac{m}{2}\dot{\underline{r}}^2 - V(\underline{r})$

$$\underline{p} = \frac{\partial L}{\partial \dot{\underline{r}}} = m\dot{\underline{r}} \qquad \left(L = \frac{m}{2}\sum_i \dot{x}_i^2 - V(\underline{r}) \quad p_i = \frac{\partial L}{\partial \dot{x}_i} = m\dot{x}_i \right)$$

b) Central force problem in polar coordinates:

$$L = \frac{m}{2}(\dot{r}^2 + r^2\dot{\varphi}^2) - U(r)$$



$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}$$

$$p_\varphi = \frac{\partial L}{\partial \dot{\varphi}} = mr^2\dot{\varphi} = L_z \quad \text{angular momentum}$$

- From $S(q,t) = \int_{t_0}^{t} dt' \, L(q(t'), \dot{q}(t'), t')$ we obtain by differentiating

$$L = \frac{dS}{dt} = \frac{\partial S}{\partial q}\dot{q} + \frac{\partial S}{\partial t} = p\dot{q} + \frac{\partial S}{\partial t}$$

- Introduce <u>Hamiltonian</u> (energy)

$$\boxed{\begin{aligned} H &= p\dot{q} - L \\ \frac{\partial S}{\partial t} &= -H \end{aligned}}$$

<u>Note</u>: The transformation from $L = L(q, \dot{q}, t)$ to $H = p\dot{q} - L = H(p, q, t)$ is a <u>*Legendre Transformation*</u>

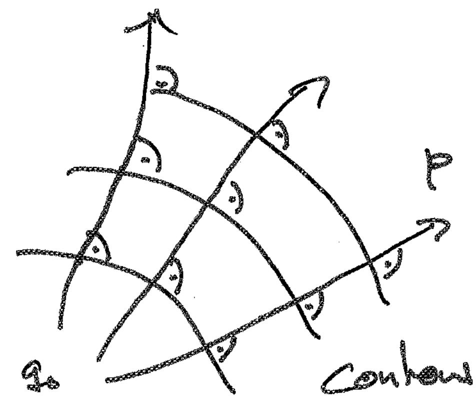
- Writing $H = H(q, p, t)$ (eliminating $\dot{q}$ by using $p = \frac{\partial L}{\partial \dot{q}}$) and using that $p = \frac{\partial S}{\partial q}$, we obtain a partial differential equation for S:

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

Hamilton-Jacobi Equation

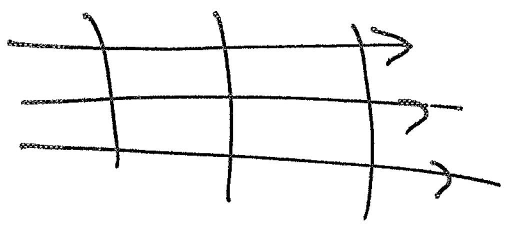
- Action waves:

$$\frac{\partial S}{\partial q} = p$$
$$= \vec{\nabla}_q S$$



contour lines of S
"wave fronts"

we can move q_0 to infinity



beam of trajectories

One solution of the Hamilton-Jacobi equation describes an entire family of trajectories and gives insight in the general behaviour.
In the next sections we will establish connections to optics and quantum mechanics

Example 1: One-dimensional motion

$L = \frac{m}{2}\dot{x}^2 - U(x)$

canonical momentum
$$\boxed{p = \frac{\partial L}{\partial \dot{x}} = m\dot{x}}$$

Hamiltonian: $\boxed{H(x,p)} = p\dot{x} - L$

$$= p\frac{p}{m} - \left(\frac{m}{2}\left(\frac{p}{m}\right)^2 - U(x)\right)$$

$$= \frac{p^2}{2m} + U(x) \qquad \text{energy}$$

Hamilton-Jacobi equation: $$\boxed{\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + U(x) = 0}$$

U is not time dependent $\Rightarrow$ Energy conserved

$$\rightarrow \boxed{S(x,t) = W(x) - Et} \qquad W(x) \equiv W_E(x) \text{ characteristic function}$$

$$\frac{1}{2m}\left(\frac{dW}{dx}\right)^2 + U(x) = E$$

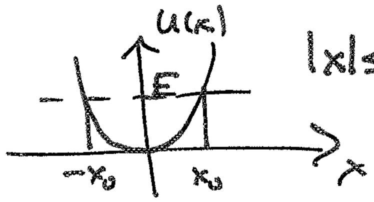
formal solution for $W(x)$:

$$\boxed{W(x) = \pm \int dx \sqrt{2m(E - U(x))}}$$

This is only real in the physically allowed region $\{x \mid U(x) \leq E\}$

Consider harmonic oscillator:

$$U(x) = \frac{k}{2}x^2, \quad \omega = \sqrt{\frac{k}{m}}$$



$|x| \leq x_0$

$$E = \frac{k}{2}x_0^2$$

$$\Rightarrow x_0 = \sqrt{\frac{2E}{k}}$$

$$\boxed{W(x)} = \pm \int dx \sqrt{2mE - mkx^2}$$

$$\underset{\xi = \sqrt{\frac{k}{2E}}\,x = x/x_0}{=} \pm \frac{2E}{\omega}\int d\xi \sqrt{1-\xi^2}$$

$$= \pm \frac{E}{\omega}\left(\xi\sqrt{1-\xi^2} + \arcsin\xi\right) \qquad (|\xi| \leq 1)$$

Only for $|\xi| = \frac{|x|}{x_0} \leq 1$, $W(x)$ is real. As we shall see when we look at the correspondence with QM shortly, complex $W(x)$ correspond to evanescent quantum waves.

Example 2: Central force problem in polar coordinates

$$L = \frac{m}{2}\left(\dot{r}^2 + r^2\dot{\varphi}^2\right) - U(r)$$

canonical momenta:

$$\boxed{\begin{aligned} p_r &= m\dot{r} \\ p_\varphi &= mr^2\dot{\varphi} \end{aligned}}$$

Hamiltonian: $\boxed{H = p\dot{q} - L} = \sum_i p_i \dot{q}_i - L$

$$= p_r\dot{r} + p_\varphi\dot{\varphi} - L$$

$$= \frac{p_r^2}{m} + \frac{p_\varphi^2}{mr^2} - \frac{m}{2}\left(\frac{p_r}{m}\right)^2 - \frac{m}{2}r^2\left(\frac{p_\varphi}{mr^2}\right)^2 + U$$

$$= \boxed{\frac{p_r^2}{2m} + \frac{p_\varphi^2}{2mr^2} + U(r)}$$

Hamilton-Jacobi equation (use $p_i = \frac{\partial S}{\partial q_i}$)

$$\boxed{\frac{\partial S}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \varphi}\right)^2\right] + U(r) = 0}$$

partial differential equation for $S(r,\varphi,t)$

First we separate time as before:

$$\boxed{S(r,\varphi,t) = W(r,\varphi) - Et}$$

$$\rightsquigarrow \boxed{\frac{1}{2m}\left[\left(\frac{\partial W}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial W}{\partial \varphi}\right)^2\right] + U(r) = E}$$

Since $U(r)$ is independent of φ, the φ dependence of $W(r,\varphi)$ is trivial (we use that $p_\varphi = \underset{\displaystyle \frac{\partial W}{\partial \varphi}}{\frac{\partial S}{\partial \varphi}} = L_z = \mathrm{const}$)

$$\boxed{W_1(r,\varphi) = W_1(r) + L_z \varphi}$$

→ remaining differential equation of 1d problem

$$\boxed{\frac{1}{2m}\left(\frac{dW_1}{dr}\right)^2 + U_{eff}(r) = E}\,, \quad \boxed{U_{eff}(r) = U(r) + \frac{L_z^2}{2mr^2}}$$

→ Formal solution: $\boxed{W_1(r) = \pm \int dr \sqrt{2m(E - U_{eff}(r))}}$

For example, in the Kepler problem $U(r) = -\frac{\alpha}{r}$, $\alpha > 0$

$$W_1(r) = \pm \int dr \sqrt{2m\left(E + \frac{\alpha}{r} - \frac{L_z^2}{2mr^2}\right)}$$

$$\underset{\substack{\boxed{r = p\varrho} \\ \boxed{p = \frac{L_z^2}{\alpha m}} \\ \text{as before}}}{=} \pm L_z \int d\varrho \sqrt{\epsilon^2 - \left(\frac{1}{\varrho} - 1\right)^2} =: \pm L_z \int d\varrho\, f(\varrho)$$

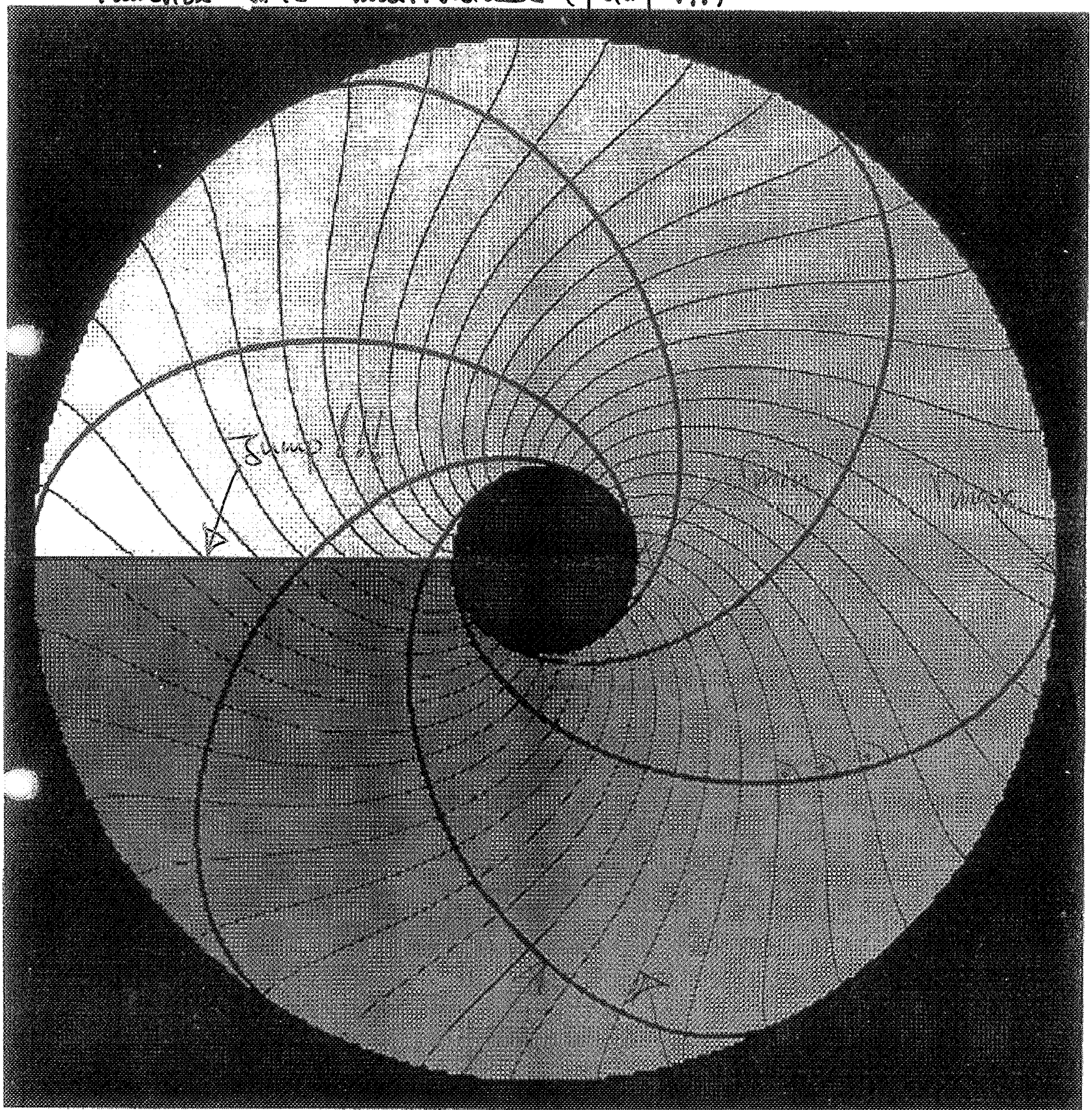
with excentricity

$$\boxed{\epsilon = \sqrt{1 + \frac{2EL_z^2}{\mu\alpha^2}}} \quad \text{as before}$$

Integral can be performed:

$$\boxed{W_1(r) = \pm L_z \left\{ \varrho f(\varrho) + \arctan\left(\frac{\varrho^{-1} - 1}{f(\varrho)}\right) - \frac{1}{\sqrt{1-\epsilon^2}} \arctan\left(\frac{\varrho^{-1} - 1 + \epsilon^2}{f(\varrho)\sqrt{1-\epsilon^2}}\right)\right\}}$$

- Contour lines of $W(\vec{x})$ for the Kepler problem with $\epsilon = 0.7$ (positive solution)
- Also shown: Trajectories which are perpendicular to contour lines and are half ellipses
- Function W is multivalued (jump!!!)



Trajectories (half ellipses)

lines of constant W

Roadmap for Hamilton-Jacobi Theory

Step 1: Establish the Lagrangian of the system

$$L = L(q, \dot{q}, t) \qquad , \quad q = (q_1, \dots, q_n)$$
$$\dot{q} = (\dot{q}_1, \dots, \dot{q}_n)$$

(pick coordinates q that reflect the symmetries of the system)

Step 2: Calculate canonical momenta

$$p = \frac{\partial L}{\partial \dot{q}} \qquad \left(p_i = \frac{\partial L}{\partial \dot{q}_i} \quad (i = 1, \dots, n) \right)$$
$$= (p_1, \dots, p_n)$$

Note: If $\frac{\partial L}{\partial q_i} = 0$: p_i conserved quantity!
(follows from Euler-Lagrange equation)

Step 3: Obtain the Hamiltonian by Legendre transformation

$$H = p\dot{q} - L = \sum_i p_i \dot{q}_i - L(q, \dot{q}, t)$$

$$\underset{\uparrow}{=} \quad H(q, p, t)$$

express $\dot{q}_i$'s by coordinates q_α and momenta p_i using $p = \frac{\partial L}{\partial \dot{q}}$

Step 4: Hamilton-Jacobi differential equation for $S(q,t)$

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

$$\Rightarrow \quad \frac{\partial S}{\partial t} + H\left(q_1, \ldots, q_n, \frac{\partial S}{\partial q_1}, \ldots, \frac{\partial S}{\partial q_n}, t\right) = 0$$

differential equation is :
- first order
- partial
- non-linear (H contains p^2 → terms $\left(\frac{\partial S}{\partial q}\right)^2$)

Step 5: Solve Hamilton-Jacobi Equation

Solution gives you $S = S(q_1, \ldots, q_n, t, \underbrace{\alpha_1, \ldots, \alpha_n}_{\text{integration constants}}) + \alpha_0$ ← trivial constant that can be dropped

How to get the solution ??

If L and H do not explicitly depend on time, Energy is conserved : $\alpha_1 = E$

$$S(q,t) = -Et + W(q)$$
$$= -Et + \underbrace{W(q_1, \ldots, q_n, \alpha_1 = E)}_{\text{characteristic function}}$$

If the problem is separable, there exists a set of coordinates $q = (q_1, \ldots, q_n)$ that

$$W(q_1, \ldots, q_n) = W_1(q_1) + \ldots W_n(q_n)$$

(e.g. parabolic coordinates in Q4/hwk 6)

→ n ordinary differential equations for $W_i(q_i)$ that are decoupled, much easier to solve

Step 6: Obtain dynamics ($q(t)$, $p(t)$)

from $\beta_i = \frac{\partial S}{\partial \alpha_i}$ $(i = 1, \ldots, n)$ and $p_i = \frac{\partial S}{\partial q_i}$ $(i = 1, \ldots, n)$

Back to Example 2: (Central force problem)

After steps 1, 2, 3, 4: Hamilton–Jacobi equation for $S(r,\varphi,t)$:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \varphi}\right)^2\right] + U(r) = 0$$

Step 5:
Hamilton and Lagrangian do not explicitly depend on time $\Rightarrow$ $\boxed{\alpha_1 = E}$ conserved

$\rightarrow$ $S(r,\varphi,t) = -Et + W(r,\varphi,E)$ $\rightarrow$ $\frac{1}{2m}\left[\left(\frac{\partial W}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial W}{\partial \varphi}\right)^2\right] + U(r) = 0$

separation ansatz: $W(r,\varphi) = W_1(r) + W_2(\varphi)$

$$\frac{1}{2m}\left(\frac{dW_1}{dr}\right)^2 + \frac{1}{2mr^2}\left(\frac{dW_2}{d\varphi}\right)^2 + U(r) = E$$

$$\frac{1}{2mr^2}\left(\frac{dW_2}{d\varphi}\right)^2 = E - U(r) - \frac{1}{2m}\left(\frac{dW_1}{dr}\right)^2$$

$$\left(\frac{dW_2}{d\varphi}\right)^2 = 2mr^2(E-U(r)) - r^2\left(\frac{dW_1}{dr}\right)^2$$

lhs depends only on φ, rhs only on r
$\Rightarrow$ both sides equal to a constant $\boxed{\alpha_2^2 = \left(\frac{dW_2}{d\varphi}\right)^2 = \left(\frac{\partial S}{\partial \varphi}\right)^2 = p_\varphi^2 = L_z^2}$

$$\Rightarrow \quad L_z^2 = 2mr^2(E-U(r)) - r^2\left(\frac{dW_1}{dr}\right)^2$$

$$\Leftrightarrow \quad \frac{L_z^2}{2mr^2} = E - U(r) - \frac{1}{2m}\left(\frac{dW_1}{dr}\right)^2$$

$\frac{dW_2}{d\varphi} = L_z$
$\Rightarrow \boxed{W_2(\varphi) = L_z\varphi}$

$$\Rightarrow \frac{dW_1(r)}{dr} = \pm\sqrt{2m}\sqrt{E - U_{eff}(r)}, \quad U_{eff}(r) = U(r) + \frac{L_z^2}{2mr^2}$$

$$W_1(r) = \pm\sqrt{2m}\int dr\,\sqrt{E - U_{eff}(r)}$$

$$\rightarrow \boxed{S(r,\varphi,t,\alpha_1 = E, \alpha_2 = L_z) = -Et + L_z\varphi \pm \sqrt{2m}\int dr\sqrt{E - U(r) - \frac{L_z^2}{2mr^2}}}$$

Step 6:

$$\beta_1 = \frac{\partial S}{\partial \alpha_1} = \frac{\partial S}{\partial E} = -t \pm \sqrt{\frac{m}{2}}\int\frac{dr}{\sqrt{E - U_{eff}(r)}}$$

$$\underset{\beta_1 = t_0}{\Leftrightarrow}\quad \boxed{t - t_0 = \pm\sqrt{\frac{m}{2}}\int\frac{dr}{\sqrt{E - U_{eff}(r)}}}$$

$$\beta_2 = \frac{\partial S}{\partial \alpha_2} = \frac{\partial S}{\partial L_z} = \varphi \pm \sqrt{\frac{L_z^2}{2m}}\int\frac{dr}{r^2\sqrt{E - U_{eff}(r)}}$$

$$\underset{\beta_2 = \varphi_0}{\Leftrightarrow}\quad \boxed{\varphi - \varphi_0 = \pm\frac{L_z}{\sqrt{2m}}\int\frac{dr}{r^2\sqrt{E - U_{eff}(r)}}}$$

Everything is consistent with previous results!

Comment: Example 2 shows that is a multivalued function (jump at $\varphi = \pi$)

$$\Rightarrow \quad \Delta W = \oint dW = \oint \left(\frac{\partial W}{\partial q} dq + \underbrace{\frac{\partial W}{\partial t} dt}_{=0} \right) = \oint p\,dq \neq 0$$

As we will see in a moment, the quantum mechanical wavefunction can be written in the semiclassical limit as

$$\psi = A\, e^{iS/\hbar} .$$

This must be single valued which implies that

$$\oint p\,dq = 2\pi\hbar \cdot n , \quad n \text{ integer}$$

$\rightarrow$ Bohr-Sommerfeld quantization

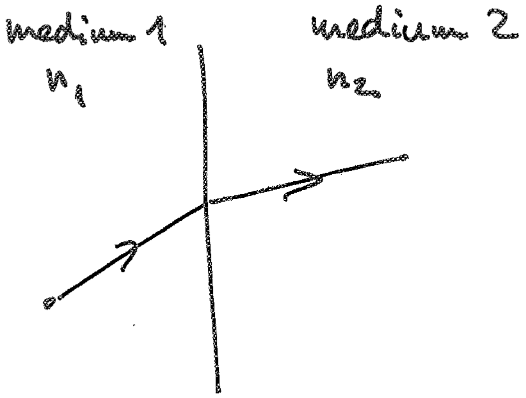
4.2. Relationship to quantum mechanics

Quantum mechanics (QM) is a theory of wavelike properties of matter. Before turning to it and having to face the quantum weirdness that comes with it, we make a brief excursion into optics.

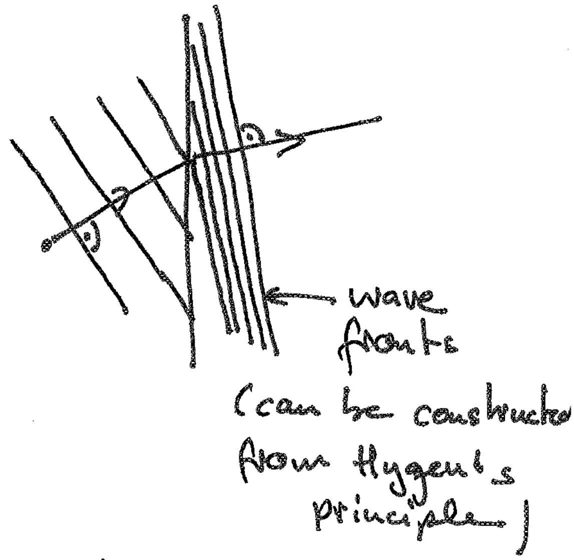
Fermat's principle: light takes the shortest optical path (fewest number of wavelength)

This is actually an action principle. It provides the relationship between ray and wave optics.

ray optics



wave optics



The light wave may be written in the form

$$u = a \cdot e^{i\phi}, \qquad \phi = \int(\underline{k}(\underline{r})\, d\underline{r} - \omega dt)$$

"action"

for plane waves: $\underline{k}, \omega$ constant, $\phi = \underline{k}\cdot\underline{r} - \omega t$

dispersion relation connects k and ω:

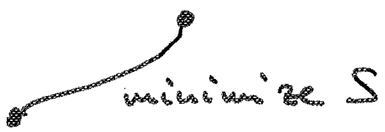
$$k = n(\underline{r})\,\frac{\omega}{c}$$

Fermat's principle: Find optimum path so that $\delta\phi = 0$

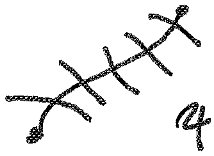
Back to QM....

- The semiclassical approximation

classical mechanics



wave mechanics



Taking the hint from what we have just seen for optics, we anticipate that the semiclassical wavefunction can be written in the form

$$\boxed{\psi = A \cdot e^{iS/\hbar}}$$

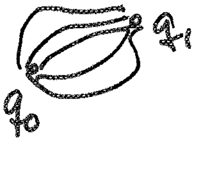
semiclassical approximation

We will see in a moment how some of our results for classical properties of S can be used to deduce a wave equation (partial differential equation) for ψ.
→ Schrödinger equation

- Broader Context: Feynman path integral

Feynman developed an entirely different approach to QM from that of Schrödinger and Heisenberg — one that is much closer in spirit to Lagrangian and Hamiltonian mechanics.

Basically, Feynman said that the wavefunction can be written as a sum over all possible path from $q_0 \to q_1$, each weighted by a complex phase $e^{iS/\hbar}$:



$$\psi(q) = \underbrace{\int \mathcal{D}q}_{\text{sum over all paths from } q_0 \text{ to } q_1} \, e^{iS/\hbar}$$

"Superposition of waves"

In the classical limit, only paths with constructive interference will contribute significantly, e.g. only paths for which S is the same and optimal, $\delta S = 0$.

$$\rightarrow \boxed{\psi = \int \mathcal{D}q \, e^{iS/\hbar} \simeq \underline{A e^{iS/\hbar} \text{ with } \delta S = 0}}$$

But $\delta S = 0$ is just the least action principle for the classical path !!!

- Deducing a wave equation for ψ: The Schrödinger equation

Differential equation must satisfy a couple of principles

1. Superposition (ψ_1, ψ_2 solutions $\Rightarrow$ $\psi_1 + \psi_2$ solution) $\Rightarrow$ differential equation must be linear
2. ψ describes state, differential equation evolution in time $\Rightarrow$ 1st order in time

We can always write such an equation in the form

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi$$

$\hat{H}$ – some linear operator whose form we must deduce

Use the ansatz $\psi = A e^{iS/\hbar}$ (semiclassical approximation) and assume that A is not changing in time.

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar \frac{i}{\hbar} \frac{\partial S}{\partial t} \psi = - \frac{\partial S}{\partial t} \psi \underset{\text{Hamilton Jacobi}}{=} \frac{1}{2m} (\nabla S)^2 \psi + U\psi$$

$(\nabla S)^2 \psi$ can be related to $\nabla^2 \psi$:

$$\nabla^2 \psi = \nabla^2 (A e^{iS/\hbar}) = \nabla ((\nabla A) e^{iS/\hbar} + A \nabla e^{iS/\hbar})$$

$$= (\nabla^2 A) e^{iS/\hbar} + 2 (\nabla A) (\nabla e^{iS/\hbar}) + A \nabla^2 e^{iS/\hbar}$$

$$= (\nabla^2 A) e^{iS/\hbar} + 2 \frac{i}{\hbar} (\nabla A)(\nabla S) e^{iS/\hbar}$$

$$- \frac{1}{\hbar^2} A (\nabla S)^2 e^{iS/\hbar} + \frac{i}{\hbar} A (\nabla^2 S) e^{iS/\hbar} \qquad (*)$$

$$\underset{\substack{\text{neglect derivatives} \\ \text{of } A \text{ an} \\ \text{2nd derivatives of } S}}{\simeq} - \frac{1}{\hbar^2} (\nabla S)^2 \psi$$

$$\Rightarrow \quad \boxed{ i\hbar \frac{\partial \psi}{\partial t} = - \frac{\hbar^2}{2m} \nabla^2 \psi + U\psi } \qquad \text{Schrödinger equation}$$

$$\boxed{ \hat{H} = - \frac{\hbar^2}{2m} \nabla^2 + U } \qquad \text{Hamiton operator}$$

- Semiclassical quantum mechanics

  we have already introduced the semiclassical wavefunction $\psi = A e^{iS/\hbar}$. Now we deduce now the <u>probability density</u> $|A|^2$ behaves

  Without loss of generality, we can assume that A is real.

$$i\hbar \frac{\partial \psi}{\partial t} = \left(i\hbar\frac{\partial A}{\partial t} - A\frac{\partial S}{\partial t}\right)e^{iS/\hbar} \underset{\text{Hamilton-Jacobi}}{=} \left(i\hbar\frac{\partial A}{\partial t} + \frac{A}{2m}(\nabla S)^2 + AU\right)e^{iS/\hbar}$$

$$\Vert$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + U\psi \underset{(*)}{=} -\frac{\hbar^2}{2m}\left(\overbrace{\nabla^2 A}^{\text{ignore}} + 2\tfrac{i}{\hbar}(\nabla A)(\nabla S) - \frac{1}{\hbar^2}A(\nabla S)^2 + \overbrace{\tfrac{i}{\hbar}A(\nabla^2 S)}^{\text{ignore}}\right)e^{iS/\hbar}$$

$$+ AUe^{iS/\hbar}$$

$$\Leftrightarrow \quad i\hbar\frac{\partial A}{\partial t} = -i\frac{\hbar}{m}(\nabla A)\underbrace{(\nabla S)}_{\underline{p}}$$

$$\Leftrightarrow \quad \frac{\partial A}{\partial t} = -\underline{v}\,\nabla A = -\frac{1}{2A}\nabla(A^2\underline{v})$$

$$\Rightarrow \quad \boxed{\frac{\partial}{\partial t}(A^2) = -\nabla(\underline{A^2\underline{v}})}$$

Continuity equation

probability density

probability current