LECTURE 36: Appendix

I. Dynamical phase of a particle is a potential

II. Constructive interference implies particle trajectories.

III. Space time history of a wave packet: Dispersion of a wave packet.

IV. Hamiltonian system; Its phase space; Hamiltonian vector field; Planck's quantum of action.

Taken from "Variational Calculus", Chap. 3,
https://people.math.osu.edu/gerlach.1/math545/
→ Lecture Notes on Variational and Tensor Calculus

PROBLEM. (*Particle in a potential*)
Set up and solve the Hamilton-Jacoby equation for a particle in a one dimensional potential $U(x)$.
Solution. Setting up the H-J equation is a three step process.

(1) Exhibit the Lagrangian:

$$L = \frac{1}{2}m\dot{x}^2 - U(x)\,.$$

(2) Determine the momentum and the Hamiltonian:

$$\begin{aligned} p &= \frac{\partial L}{\partial \dot{x}} \\ &= m\dot{x}\,; \\ H &= \dot{x}\frac{\partial L}{\partial \dot{x}} - L \\ &= \frac{1}{2}m\dot{x}^2 + U(x)\,. \end{aligned}$$

(3) Express the Hamiltonian in terms of the momentum:

$$H = \frac{p^2}{2m} + U(x)\,.$$

(4) Write down the H-J equation $-\frac{\partial S}{\partial t} = H\left(x, \frac{\partial S}{\partial x}\right)$:

$$-\frac{\partial S}{\partial t} = \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + U(x)\,.$$

This a first order non-linear partial differential equation that needs to be solved for the scalar function $S(x,t)$.
This p.d.e. lends itself to being solved by the method of separation of variables according to which one finds solutions of the form

$$S(x,t) = T(t) + X(x)\,. \tag{3.5.7}$$

Introducing this form into the H-J equation, one finds

$$-\frac{dT(t)}{dt} = \frac{1}{2m}\left(\frac{dX(x)}{dx}\right)^2 + U(x)\,.$$

This equation says that the left hand side is independent of x, while the right hand side is independent of t. Being equal, the l.h.s. is also independent of x. Being independent of both t and x, it is a constant. Letting this "separation" constant be equal to E, one obtains two equations

$$\begin{aligned} -\frac{dT(t)}{dt} &= E \\ \frac{1}{2m}\left(\frac{dX(x)}{dx}\right)^2 + U(x) &= E\,. \end{aligned}$$

These are two ordinary equations for T and X. Inserting these equations into Eq. (3.5.7), one obtains the sought after solution to the H-J equation,

$$S(x,t) = -Et + \int^x \sqrt{2m\,(E - U(x'))}\,dx' + \delta(E)\,.$$

Here the "integration constant" $\delta(E)$ is an arbitrary function of E. Furthermore, observe that S depends on E also. This means that one has an E-parametrized family of solutions. Thus, properly speaking, separation of variables yields many solutions to the H-J equation, in fact, a one-parameter family of them

$$S(x,t) = S_E(x,t) .$$

3.5.2. Several Degrees of Freedom. We shall see in a subsequent section that whenever the H-J for a system with several degrees of freedom, say $\{q^i\}$, lends itself to being solved by the method of the separation of variables, i.e.

$$S(q^i,t) = T(t) + \sum_{i=1}^{s} Q_i(q^i) ,$$

the solution has the form

$$S = -\int^t E dt + \sum_{i=1}^{s} \int^{q^i} p_i(x^i; E, \alpha_1, \cdots, \alpha_{s-1}) dq^i + \delta(E, \alpha_1, \cdots, \alpha_{s-1})$$

Here δ is an arbitrary function of E and the other separation constants that arise in the process of solving the H-J equation. We see that for each choice of $(E, \alpha_1, \cdots, \alpha_{s-1})$ we have a different solution S. Thus, properly speaking, we have $S_{E,\alpha_1,\cdots,\alpha_{s-1}}$, a multi-parametrized family of solutions to the H-J equation.

We shall now continue our development and show that Hamilton-Jacobi Theory is

a) A new and rapid way of integrating the E-L equations

b) The bridge to wave (also "quantum") mechanics.

The virtue of Hamilton's principle is that once the kinetic and potential energy of the system are known, the equations of motion can be set up with little effort. These Euler-Lagrange equations are Newton's equations of motion for the system. Although setting up the equations of motion for a system is a routine process, solving them can be a considerable challenge. This task can be facilitated considerably by using an entirely different approach. Instead of setting up and solving the set of coupled Newtonian ordinary differential equations, one sets up and solves a single partial differential equation for a single scalar function. Once one has this scalar function, one knows everything there is to know about the dynamical system. In particular, we shall see that by differentiating this scalar function (the dynamical phase, the Hamilton-Jacobi function, the eikonal) one readily deduces all possible dynamical evolutions of the system.

3.6. Hamilton-Jacobi Description of Motion

Hamilton-Jacobi theory is an example of the *principle of unit economy*[3], according to which one condenses a vast amount of knowledge into a smaller and smaller number of principles. Indeed, H-J theory condenses all of classical mechanics and all of wave mechanics (in the asymptotic high-frequency/short-wavelength (a.k.a. W.K.B.) approximation) into two conceptual units,, (i) the H-J equation

[3]The *principle of unit economy*, also known informally as the "crow epistemology", is the principle that stipulates the formation of a new concept

(1) when the description of a set of elements of knowledge becomes too complex,

(2) when the elements comprising the knowledge are used repeatedly, and

(3) when the elements of that set require further study.

Pushing back the frontier of knowledge and successful navigation of the world demands the formation of a new concept under any one of these three circumstances.

and (ii) the principle of constructive interference. These two units are a mathematical expression of the fact that classical mechanics is an asymptotic limit of wave mechanics.

Hamilton thinking started with his observations of numerous known analogies between "particle world lines" of mechanics and "light rays" of geometric optics. These observations were the driving force of his theory. With it he developed classical mechanics as an asymptotic limit in the same way that ray optics is the asymptotic limit of wave optics. Ray optics is a mathematically precise asymptotic limit of wave optics. Hamilton applied this mathematical formulation to classical mechanics. He obtained what nowadays is called the Hamilton-Jacobi formulation of mechanics. Even though H-J theory is a mathematical limit of wave mechanics, in Hamilton's time there was no logical justification for attributing any wave properties to material particles. (That justification did not come until experimental evidence to that effect was received in the beginning of the 20th century.) The most he was able to claim was that H-J theory is a mathematical method with more unit economy than any other formulation of mechanics. The justification for associating a wave function with a mechanical system did not come until observational evidence to that effect was received in the beginning of the 20th century.

We shall take advantage of this observation (in particular by Davidson and Germer, 1925) implied association by assigning to a mechanical system a wave function. For our development of the H-J theory it is irrelevant whether it satisfies the Schroedinger, the Klein-Gordon, or some other quantum mechanical wave equation. Furthermore, whatever the form of the wave equation governing this wave function, our focus is only on those circumstances where the wave function has the form

$$\Psi_E(x,t) = \underbrace{\mathcal{A}(x,t)}_{\textit{slowly}\text{ varying function of } x \text{ and } t} \times \underbrace{\exp\left(\frac{i}{\hbar}S_E(x,t)\right)}_{\textit{rapidly}\text{ varying function of } x \text{ and } t} \tag{3.6.1}$$

This circumstance is called the "high frequency" limit or the "semi-classical" approximation. It can be achieved by making the energy E of the system large enough. In that case

$$1 << \frac{S_E(x,t)}{\hbar}$$

with the consequence that the phase factor oscillates as a function of x and t rapidly indeed. The existence of such a wave function raises a non-trivial problem:
If the wave and its dynamical phase, and hence the wave intensity, is defined over all of space-time, how is it possible that a particle traces out a sharp and well defined path in space-time when we are left with three delemas?

(1) The large magnitude ($S \gg \hbar$=1.05×10^{-27}[erg sec]) of the action for a classical particle is certainly of no help.

(2) Neither is the simplicity of the H-J equation

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

which governs the dynamical phase in

$$\Psi = \mathcal{A}\exp\left(i\frac{S}{\hbar}\right),$$

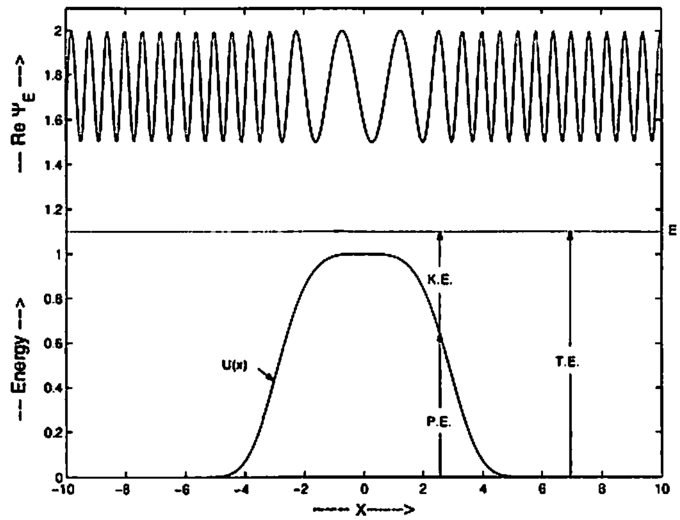

FIGURE 3.6.1. The spatial oscillation rate of the wave function $Re\,\Psi_E$ at $t = const.$ is proportional to its x-momentum, whose square is proportional to the kinetic energy (K.E.=T.E.-P.E.).

(3) Nor is the simplicity of the solution S for a particle of energy E,

$$S(x,t) = -Et + \int_{x_o}^{x} \sqrt{2m(E - U(x))}dx + \delta(E)$$

of any help in identifying a localized trajectory ("world line") of the particle in space-time coordinatized by x and t.

What *is* of help is the basic implication of associating a wave function with a moving particle, namely, it is a linear superposition of monochromatic waves, Eq. (3.6.1), which gives rise to a travelling wave packet – a localized moving wave packet whose history is the particle's world line. To validate this claim we shall give two heuristic arguements (i-ii), one application (iii), a more precise argument (iv) and an observation (v).

(i): The most elementary superposition monochomatic waves is given by the sum wave trains with different wavelengths

$$\Psi(x,t) = \Psi_E(x,t) + \Psi_{E+\Delta E}(x,t) + \cdots .$$

(ii): In space-time one has the following system of level surfaces for $S_E(x,t)$ and $S_{E+\Delta E}(x,t)$

Destructive interference between different waves comprising Ψ(x,t) occures everywhere except where the phase of the waves agree:

$$S_E(x,t) = S_{E+\Delta E}(x,t)$$

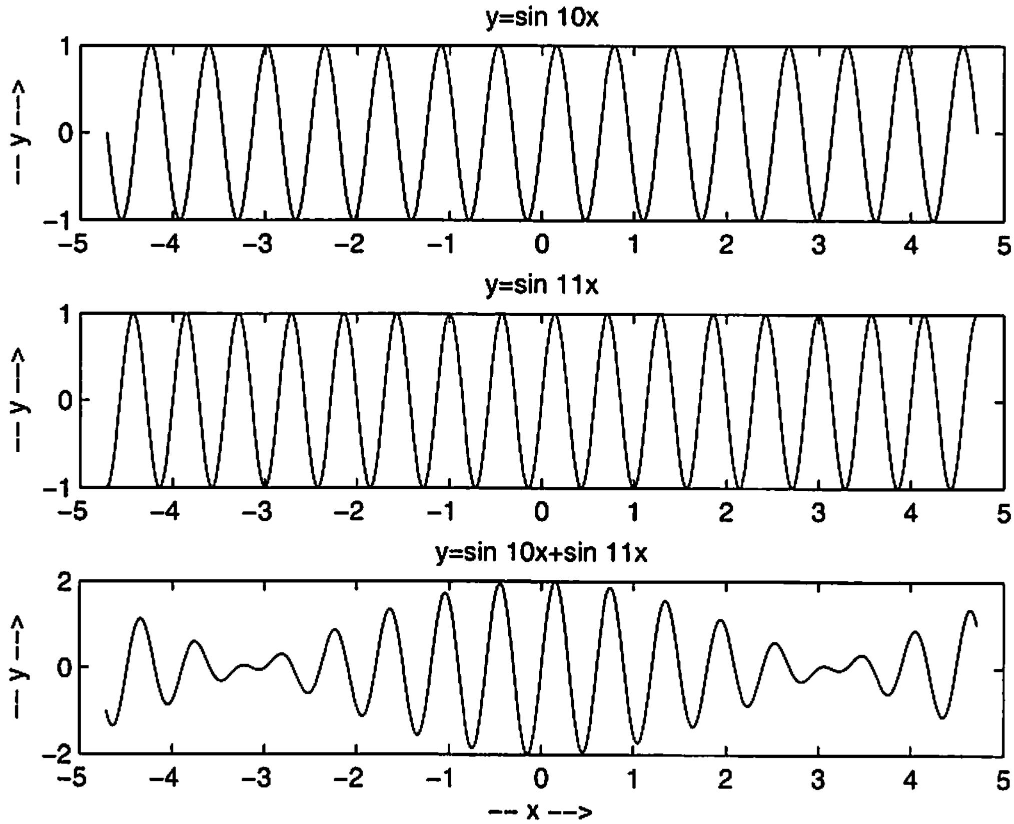

FIGURE 3.6.2. Photographic snapshot in space of two interfering wave trains and their resulting wave packet.

At the locus of events satisfying this condition, the waves interfere constructively and wave packet has non-zero amplitude. The quantum priciple says that this condition of constructive interference

$$0 = \lim_{\Delta E \to 0} \frac{S_{E+\Delta E}(x,t) - S_E(x,t)}{\Delta E} = \frac{\partial S_E(x,t)}{\partial E}$$

yields a Newtonian worldline, i.e. an extremal paths.

(iii): Apply this condition to the action S(x,t) of a single particle. One obtains the time the particle requires to travel to point x,

$$0 = -t + \int_{x_0}^{x} \sqrt{\frac{m}{2}} \left(\frac{1}{E - U(x)} \right)^{\frac{1}{2}} dx + t_0$$

with

$$t_0 \equiv \frac{\partial \delta(E)}{\partial E} .$$

This condition yields the Newtonian worldline indeed. The precise arguement is Lecture 13. The additional observation is on p13 Lecture 13.

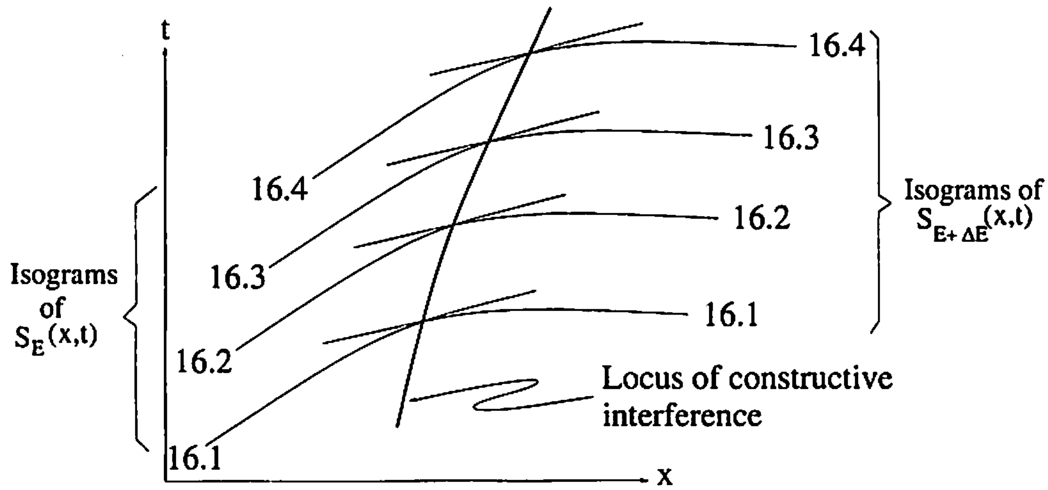

FIGURE 3.6.3. Constructive interference represented in spacetime. The intersection of the respective isograms of $S_E(x,t)$ and $S_{E+\Delta E}(x,t)$ locates the events (x,t) which make up the trajectory of the particle in x-t space – the locus of constructive interference.

Lecture 13

Wave Packets via 3.7. Constructive Interference

Our formulation of constructive interference is based on a picture in which at each time t a superposition of wave trains

$$\Psi_E(x,t) + \Psi_{E+\Delta E}(x,t) + \cdots \equiv \Psi(x,t)$$

yields a wave packet at time t. The principle of constructive interference itself,

$$\frac{\partial S_E(x,t)}{\partial E} = 0$$

is a condition which at each time t locates where the maximum amplitude of the wave packet is.
It is possible to bring into much sharper focus the picture of superposed wave trains and thereby not only identify the location of the resultant wave packet maximum, but also width of that packet.

3.8. Spacetime History of a Wave Packet

The sharpened formulation of this picture consists of replacing a *sum* of superposed wave amplitudes with an *integral* of wave amplitudes

$$\begin{aligned} \Psi(x,t) &= \text{"}\Psi_E(x,t) + \Psi_{E+\Delta E}(x,t) + \cdots\text{"} \\ &= \int_{-\infty}^{\infty} f(E)\, e^{\frac{i}{\hbar}S_E(x,t)} dE\,. \qquad S_E \end{aligned} \tag{3.8.1}$$

A very instructive example is that of a superpostion of monochromatic ("single energy") wavetrains, each one weighted by the amplitude $f(E)$ of a Gaussian window in the Fourier ("energy") domain,

$$\boxed{f(E) = Ae^{-(E-E_0)^2/\epsilon^2}} \tag{3.8.2}$$

The dominant contribution to this integral comes from within the window, which is centered around the location of E_0 of the Gaussian maximum and has width 2ϵ, which is small for physical reasons. Consequently, it suffices to represent the phase function as a Taylor series around that central point E_0, namely

(3.8.3)

$$S_E(x,t) = S_{E_0}(x,t) + \left.\frac{\partial S_E(x,t)}{\partial E}\right|_{E_0}(E-E_0) + \frac{1}{2}\left.\frac{\partial^2 S_E(x,t)}{\partial E^2}\right|_{E_0}(E-E_o)^2 + \begin{matrix}\text{higher}\\ \text{order}\\ \text{terms}\end{matrix},$$

and neglect the higher order terms. Keeping only the first three terms and ignoring the remainder allows an exact evaluation of the Gaussian superposition integral. This evaluation is based on the following formula

$$\int_{-\infty}^{\infty} e^{\alpha z^2+\beta z}dz = \sqrt{\frac{\pi}{-\alpha}}e^{-\frac{\beta^2}{4\alpha}}. \tag{3.8.4}$$

Applying it to the superpostion integral, Eq. (3.8.1) together with Eqs. (3.8.2) and (3.8.3), we make the following identification

$$\begin{aligned} z =& E - E_0\,; \quad dz = dE\,, \\ \alpha =& -\frac{1}{\epsilon^2} + \frac{i}{\hbar}\frac{1}{2}\left.\frac{\partial^2 S_E(x,t)}{\partial E^2}\right|_{E_0} \equiv -\frac{1}{\epsilon^2}(1-i\sigma)\,, \\ -\frac{1}{\alpha} =& \frac{\epsilon^2}{1-i\sigma} = \epsilon^2\frac{1+i\sigma}{1+\sigma^2}\,, \\ \sigma =& \frac{1}{2}\frac{1}{\hbar}\left.\frac{\partial^2 S_E(x,t)}{\partial E^2}\right|_{E_0}\epsilon^2\,, \\ \beta =& \frac{i}{\hbar}\left.\frac{\partial^2 S_E(x,t)}{\partial E^2}\right|_{E_0}. \end{aligned} \tag{3.8.5}$$

Inserting these expressions into the righthand side of the formula (3.8.4), one obtains

$$\begin{aligned} \Psi(x,t) &= A\sqrt{\pi}\epsilon\sqrt{\frac{1+i\sigma}{1+\sigma^2}}\exp\left\{-\frac{1}{4}\left(\frac{\frac{\partial S(x,t)}{\partial E_o}}{\hbar}\right)^2\epsilon^2\left(\frac{1+i\sigma}{1+\sigma^2}\right)\right\}e^{i\frac{S_{E_0}(x,t)}{\hbar}} \\ &\equiv \underbrace{\mathcal{A}(x,t)}_{\substack{\text{slowly}\\ \text{varying}}}\underbrace{e^{\frac{iS_{E_0}(x,t)}{\hbar}}}_{\substack{\text{rapidly}\\ \text{varying}}}. \end{aligned}$$

This is a *rapidly oscillating* function

$$e^{i\,S_{E_0}(x,t)/\hbar}$$

modulated by a *slowly varying* amplitude $\mathcal{A}(x,t)$. For each time t this product represents a wave packet. The location of the maximum of this wave packet is given implicitly by

$$\left.\frac{\partial S_E(x,t)}{\partial E}\right|_{E_0} = 0\,. \tag{3.8.6}$$

As t changes, the x-location of the maximum changes. Thus we have curve in x-t space of the locus of those events where the slowly varying amplitude $\mathcal{A}$ has a maximum. In other words, this wave packet maximum condition locates those events (= points in spacetime) where constructive interference takes place.

A wave packet has finite extent in space and in time. This extent is governed by its squared modulus, i.e. the squared magnitude of its slowly varying amplitude,

$$|\Psi(x,t)|^2 = |\mathcal{A}|^2 = A^2\pi\epsilon^2\frac{1}{\sqrt{1+\sigma^2}}\exp\underbrace{\left\{-\frac{\epsilon^2}{2}\frac{1}{\sqrt{1+\sigma^2}}\frac{\left(\frac{\partial S_E(x,t)}{\partial E}\Big|_{E_0}\right)^2}{\hbar^2}\right\}}_{\mathbf{E}(x,t)} \tag{3.8.7}$$

We see that this squared amplitude has nonzero value even if the condition for constructive interference, Eq.(3.8.6), is violated. This violation is responsible for the finite width of the wave packet. More precisely, its shape is controlled by the exponent $\mathrm{E}(x,t)$,

$$\mathrm{E}(x,t) \equiv \left\{-\frac{\epsilon^2}{2}\frac{1}{\sqrt{1+\left(\frac{\epsilon^2}{2\hbar}\frac{\partial^2 S_E(x,t)}{\partial E^2}\Big|_{E_0}\right)^2}}\frac{\left(\frac{\partial S_E(x,t)}{\partial E}\Big|_{E_0}\right)^2}{\hbar^2}\right\} \neq 0\,.$$

The spacetime evolution of this shape is exhibited in Figure 3.8.1 on the next page. Thus the worldline of the particle is not a sharp one, but instead has a slight spread in space and in time. How large is this spread?
The magnitude of the wave mechanical ("non-classical") spread in the world line is the width of the Gaussian wave packet. This spread is Δx, the amount by which one has to move away from the maximum in order that the amplitude profile change by the factor $e^{\frac{1}{2}}$ from the maximum value. Let us calculate this spread under the circumstance where the effect due to dispersion is a minimum, i.e. when σ is neglegibly small. In that case the condition that $\mathbf{E}(x+\Delta x,t) = -1$ becomes

$$\left|\frac{\epsilon}{\hbar}\frac{\partial S_E(x+\Delta x,t)}{\partial E}\Big|_{E_0}\right| = 1\,.$$

Expand the left hand side to first order, make use of the fact that (x,t) is a point in spacetime where the wavepacket profile has a maximum, i.e. satisfies Eq.(3.8.6). One obtains

$$\left|\epsilon\frac{\partial^2 S}{\partial E\partial x}\Delta x\right| = \hbar$$

or, in light of $\partial S_E(x,t)/\partial x \equiv p(x,t;E)$,

$$\left|\epsilon\frac{\partial p}{\partial E}\Delta x\right| = \hbar\,,$$

and hence

$$\boxed{\Delta p\Delta x = \hbar}$$

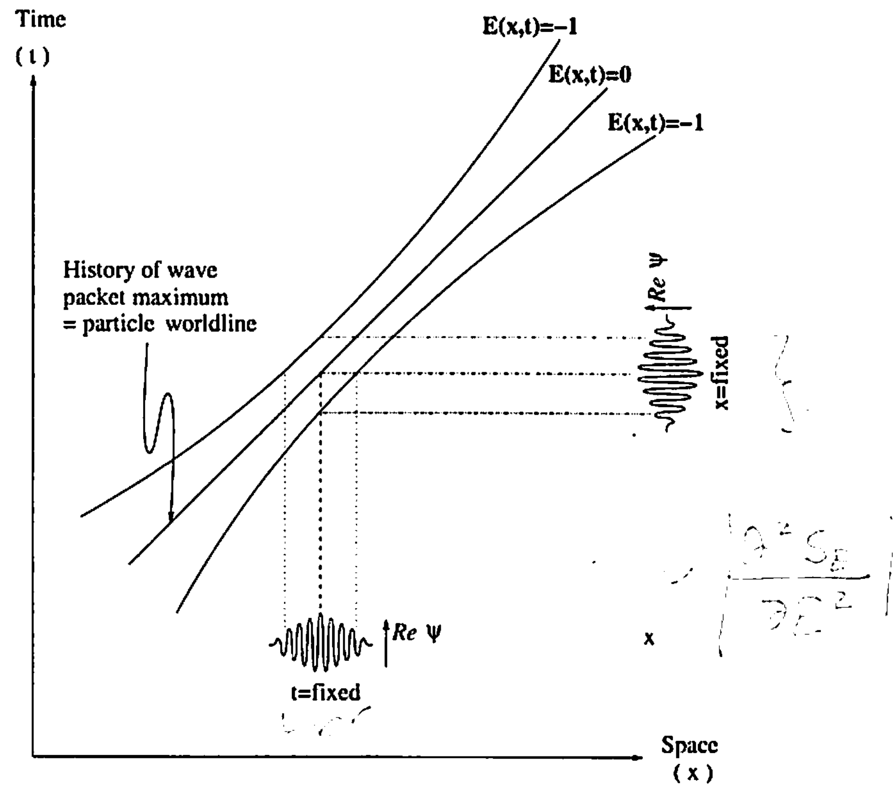

FIGURE 3.8.1. Spacetime particle trajectory ("the $\mathrm{E}(x,t)=0$ isogram") and the dispersive wave packet amplitude histories surrounding it. The two mutually diverging ones (both characterized by $\mathrm{E}(x,t)=-1$) in this figure refer to the front and the back end of the wave packet at each instant $t = fixed$, or to the beginning and the end of the wave disturbance passing by a fixed location $x = fixed$. The particle and the wave packet maximum are moving with a velocity given by the slope of the $\mathrm{E}(x,t)=0=\left.\frac{\partial S_E(x,t)}{\partial E}\right|_{E_0}$ isogram, which is the locus of constructive interference exhibited in Figure 3.6.3

On the other hand, the convergence and subsequent divergence ("dispersion") of the wave packet is controlled (and expressed mathematically) by the behavior of the second derivative, $\left.\frac{\partial^2 S_E(x,t)}{\partial E^2}\right|_{E_0}$ of the dynamicāl phase $S_E(x,t)$. Whereas the behavior of its first derivative characterizes the difference in the motion of particles launched with difference initial conditions, its second derivative characterizes the intrinsically wave mechanical aspects of each of these particles.

Similarly the temporal extent Δt, the amount by which one has to wait (at fixed x) for the wave amplitude profile to decrease by the factor $e^{-1/2}$ from its maximum value, satisfies the condition

$$\left| \frac{\epsilon}{\hbar} \frac{\partial S_E(x, t+\Delta t)}{\partial E}\bigg|_{E_0} \right| = 1$$

which become

$$\left| \epsilon \frac{\partial^2 S_E}{\partial E \partial t}\bigg|_{E_0} \Delta t \right| = \hbar$$

$$\left| \epsilon(-) \frac{\partial E}{\partial E}\bigg|_{E_0} \Delta t \right| = \hbar$$

or

$$\boxed{\Delta E \Delta t = \hbar} .$$

The two boxed equation are called the Heisenberg indeterminacy relation. Even though we started with the dynamical phase S (see page 38) with $\Psi \sim e^{\frac{iS}{\hbar}}$ to arrive at the extremal path in spacetime, the constant $\hbar$ ("quantum of action") never appeared in the final result for the spacetime trajectory. The reason is that in the limit

$$\frac{S}{\hbar} \to \infty$$

the location of the wave packet reduces to the location of the wave crest. Once one knows the dynamical phase $S(x,t)$ of the system, the condition of constructive interference gives *without approximation* the location of the sharply defined Newtonian world line, the history of this wave crest, an extremal path through spacetime.

3.9. Hamilton's Equations of Motion

To validate the claim that constructive interference leads to the extremal paths determined by the E-L equations, one must first recast them into a form that involves only q^i and p_j instead of $q^i$and $\dot{q}^j$. Holding off that validation until Section 3.11 on page 59, we achieve the transition from $(q^i, \dot{q}^j)$ to (q^i, p_j) as follows: The Lagrangian is a function of $q^i$and $\dot{q}^i$. Consequently,

$$dL = \sum_i \frac{\partial L}{\partial q^i} dq^i + \sum_i \frac{\partial L}{\partial \dot{q}^i} d\dot{q}^i$$

which may be rewritten as

$$dL = \sum_i \dot{p}_i dq^i + \sum_i p_i d\dot{q}^i ,$$

where

$$p_i = \frac{\partial L}{\partial \dot{q}^i}$$

and

$$\dot{p}_i = \frac{\partial L}{\partial q^i}$$

by the E-L equations. Using the fact that

$$p_i d\dot{q}^i = d(p_i \dot{q}^i) - \dot{q}^i dp_i ,$$

one obtains, after a sign reversal, an expression which depends only on q^i and p_i:

$$\underbrace{d\left(\sum_i p_i\dot{q}^i - L\right)}_{H} = -\sum_i \dot{p}_i dq^i + \sum_i \dot{q}^i dp_i . \tag{3.9.1}$$

Introduce the Hamiltonian of the system

$$H(p,q,t) \equiv \sum p_i\dot{q}^i - L .$$

Compare its differential

$$dH = \frac{\partial H}{\partial q^i}dq^i + \frac{\partial H}{\partial p_i}dp_i + zero \times d\dot{q}^i$$

with the one given above by Eq.(3.9.1). Recall that two differentials are equal if and only if the coefficients of the (arbitrary) coordinate differences (i.e. $dq^1, \cdots, dq^s$, $dp_1, \cdots, dp_s$) are equal. Consequently, one has

$$\boxed{\dot{q}^i = \frac{\partial H}{\partial p_i}, \qquad p_i = -\frac{\partial H}{\partial q_i}.}$$

These are the *Hamilton's* or the *canonical equations of motion.* They are equivalent to those of E-L. Comment 1: The fact that H does not depend on $\dot{q}^i$ follows directly from

$$\frac{\partial H}{\partial \dot{q}^i} = p_i - \frac{\partial L}{\partial \dot{q}^i} = 0$$

Comment 2: a) It follows from Hamilton's equations of motion that

$$\begin{aligned} \frac{dH}{dt} &= \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial p_i}\dot{p}_i + \frac{\partial H}{\partial t} \\ &= \frac{\partial H}{\partial t} \end{aligned}$$

In other words, if H is independent of any *explicit* time dependence, i.e. time then H *is a constant* along the trajectory of the evolving system.
Comment 2: b.) If H is independent of the *generalized coordinate* q^k, then

$$\frac{dp^k}{dt} = 0$$

i.e. p_k *is a constant* for the evolving system.

3.10. The Phase Space of a Hamiltonian System

The 2s-dimentional spaced is spanned by the coordinates

$$[q^1, \cdots, q^s, p_1, \cdots, p_s]$$

is called the phase space of the system. In this phase space, the curve

$$[q^i(t), p_i(t)]$$

is an integral curve of the Hamiltonian or phase path vector field

$$\left(\frac{\partial H(q,p)}{\partial p_i}, -\frac{\partial H(q,p)}{\partial q^i}\right)$$

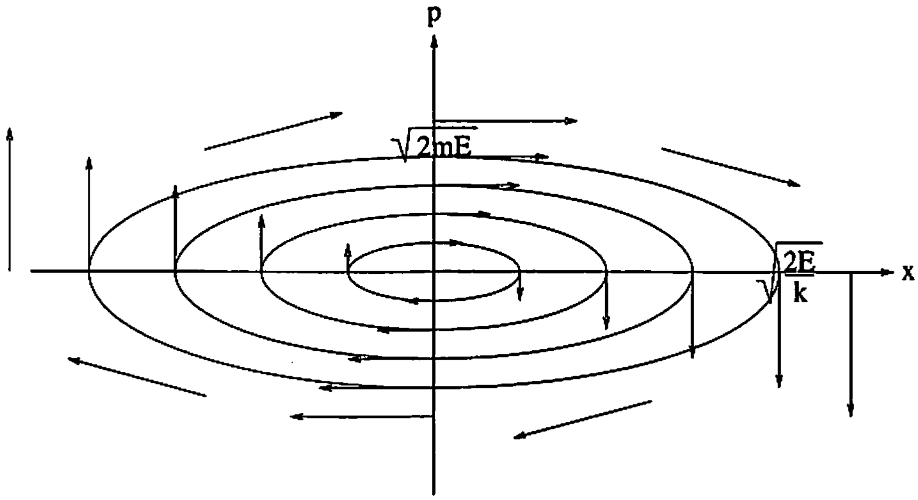

FIGURE 3.10.1. Hamiltonian vector field of a simple harmonic oscillator (s.h.o.) of mass m and spring constant k. The ellipses are integral curves whose tangents at each point are the vectors of that field. The major axis, $\sqrt{\frac{2E}{k}}$, and the minor axis, $\sqrt{2mE}$, of each ellipse are determined by the energy E of the s.h.o. The area of any particular ellipse is $2\pi E \frac{m}{k}$.

In other words, the tangents to this curve are given by

$$(\dot{q}^i, \dot{p}_i) = \left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i}\right)$$

Example: For the simple harmonic oscilator
the Lagarangian is:

$$L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2$$

and the Hamiltonian is:

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2 = E$$

a) The phase space of this system is spanned by x and p.
The Hamiltonian vector field is

$$\left(\frac{\partial H}{\partial p_i}, -\frac{\partial H}{\partial q^i}\right) = \left(\frac{p}{m}, -kx\right)$$

b) The area of one of the phase-path ellipses is

$$\text{area} = \int p dx \qquad \text{and it has the dimension of "action"}$$

According to quantum mechanics the action of a periodic system must obey the Bohr quantization condition

$$\int p dx = \left(n + \frac{1}{2}\right) h, \qquad n = 1, 2, \cdots \tag{3.10.1}$$

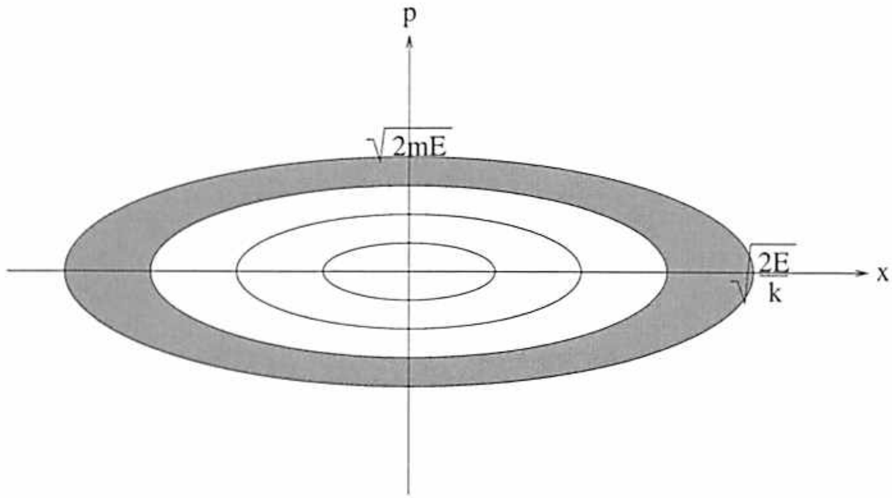

FIGURE 3.10.2. The shaded difference between the areas of adjacent phase space ellipses, Eq.(3.10.1), is precisely $h = 6.27\times10^{-27}$erg sec, which is one quantum of action.

Thus, as depicted in Figure 3.10.2, the quantum mechanically allowed phase space ellipses differ in area from one another by precisely $h = 6.27\times10^{-27}$erg sec, which is one quantum of action.

For the simple harmonic oscilator the area of one of these ellipses is $\int pdx = \pi\sqrt{2mE}\sqrt{\frac{2E}{k}} = 2\pi E\sqrt{\frac{m}{k}} = 2\pi\frac{E}{\omega}$. Thus the Bohr quantization condition yields

$$2\pi\frac{E}{\omega} = \left(n + \frac{1}{2}\right)h$$

or with $\frac{\omega}{2\pi} = frequency$

$$E = (n + \frac{1}{2})h \times frequency$$

3.11. Consturctive interference ⇒ Hamilton's Equations

The principle of constructive interference provides the bridge between particle and wave mechanics. This fact is validatede by the following theorem.

THEOREM. *Constructive interference conditions imply the Hamilton's equantions of motion and hence determine the existence of an extremal path.*

Proof: Step 1.) Consider a complete integral of the H-J equation

$$S = S(t, q^1, \cdots, q^s, \alpha_1, \cdots, \alpha_s)$$

i.e. a solution which has as many arbitrary constants as there are independent coordinates[4]. The constructive interference conditions are

$$\frac{\partial S}{\partial \alpha_k} = 0 \qquad k = 1, \cdots, s$$

They determine implicitly a trajectory $q^i = q^i(t)$, $i = 1, \cdots, s$.
Step 2.) Take the total derivative and obtain

$$\begin{aligned} 0 &= \frac{d}{dt}\frac{\partial S}{\partial \alpha_k} = \frac{\partial^2 S}{\partial t \partial \alpha_k} + \frac{\partial^2 S}{\partial q^i \partial \alpha_k}\frac{dq^i}{dt} \\ &= -\frac{\partial}{\partial \alpha_k} H(q, \frac{\partial S(t,q,\alpha)}{\partial x^i}, t) + \frac{\partial^2 S}{\partial q^i \partial \alpha_k}\frac{dq^i}{dt} \\ &= -\frac{\partial H}{\partial p_i}\frac{\partial^2 S}{\partial \alpha_k \partial q^i} + \frac{\partial^2 S}{\partial q^i \partial \alpha_k}\frac{dq^i}{dt} \\ &= \frac{\partial^2 S}{\partial \alpha_k \partial q^i}\left(\frac{dq^i}{dt} - \frac{\partial H}{\partial p_i}\right), \end{aligned}$$

which implies the 1st half of Hamilton's equations,

$$\frac{dq^i}{dt} = \frac{\partial H}{\partial p_i},$$

provided $\frac{\partial^2 S}{\partial \alpha_k \partial q^i}$ is non-singular.
Step 3.) Differentiate both sides of the H-J equation

$$\begin{aligned} 0 &= \frac{\partial}{\partial q^i}\left[\frac{\partial S}{\partial t} + H\left(q, \frac{\partial S}{\partial q}, t\right)\right] \\ &= \frac{\partial}{\partial t}\frac{\partial S}{\partial q^i} + \left.\frac{\partial H}{\partial p_k}\right)_q \frac{\partial^2 S}{\partial q^k \partial q^i} + \left.\frac{\partial H}{\partial q^i}\right)_p \\ &= \frac{\partial}{\partial t}\frac{\partial S}{\partial q^i} + \frac{dq^k}{dt}\frac{\partial}{\partial q^k}\left(\frac{\partial S}{\partial q^i}\right) + \left.\frac{\partial H}{\partial q^i}\right)_p \\ &= \frac{d}{dt}p_i + \frac{\partial H}{\partial q^i} \end{aligned}$$

which is the 2nd half of Hamilton's equation's,

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}.$$

QED. Thus the two Hamilton's equations of motion are implied by the principle of constructive interference indeed.

Lecture 14

3.12. Applications

Two of the most important applications of Hamilton-Jacobi theory are found in

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[4]Such independence is expressed mathematically by the fact that

$$det\left|\frac{\partial^2 S}{\partial q^i \partial \alpha_j}\right| \neq 0.$$

This condition would be violated if the dependence on two constants were of the form $S(t, q^i, f(\alpha_1, \alpha_2), \alpha_3, \cdots, \alpha_s)$.

(i) the motion of bodies on the astronomical scale, for example, space craft, comets, or planets moving in a gravitational field, and in.

(ii) the motion of bodies on the atomic scale, for example, a charged particle (electron) moving in the potential of an atomic nucleus or in th electromagnetic field of a pulsed laser.

The mathematical procedure for these and numerous other examples is routine and always the same:
(i) Construct the Hamiltonian for the system
(ii) Write down and solve the H-J equation
(iii) Apply the conditions of constructive interference to obtain the trajectories of the body.
Let us describe how this three step procedure is done in practice.

3.12.1. H-J Equation Relative to Curvilinear Coordinates. In constructing the Hamiltonian one must choose some specific set of coordinates. For a single particle it is is difficult to find an easier way of writing down the H-J equation than the way whose starting point is the element of arclength

$$\begin{aligned} (ds)^2 &= dx^2 + dy^2 + dz^2 \quad \text{(Cartesian coordinates)} \\ &= g_{ij}dx^i dx^j \qquad \text{(curvilinear coordinates)} \end{aligned} \tag{3.12.1}$$

This element of arclength is the best starting point because it is related so closely to the Lagrangian of the system. Indeed, one has

$$\begin{aligned} L &= \frac{1}{2}m\vec{\dot{x}}\cdot\vec{\dot{x}} - U \\ &= \frac{1}{2}m\left[\left(\frac{dx}{dt}\right)^2 + \left(\frac{dy}{dt}\right)^2 + \left(\frac{dz}{dt}\right)^2\right] - U \\ &= \frac{1}{2}m\, g_{ij}\frac{dx^i}{dt}\frac{dx^j}{dt} - U\,. \end{aligned}$$

In other words, the Lagrangian is constructed relative to curvilinear coordinates by inspection. The steps leading to the H-J equation are now quite routine.

The momenta are

$$p_j = \frac{\partial L}{\partial \dot{x}^j} = m\, g_{ij}\dot{x}^i\,.$$

Let g^{kj}be the inverse of g_{ji}: $g^{kj}g_{ji} = \delta^k_i$ so that

$$\dot{x}^i = \frac{1}{m}g^{ij}p_j$$

and

$$H = p_j\dot{x}^j - L = \frac{1}{2m}g^{ij}p_ip_j + U$$

Thus the Hamilton-Jacobi equation is

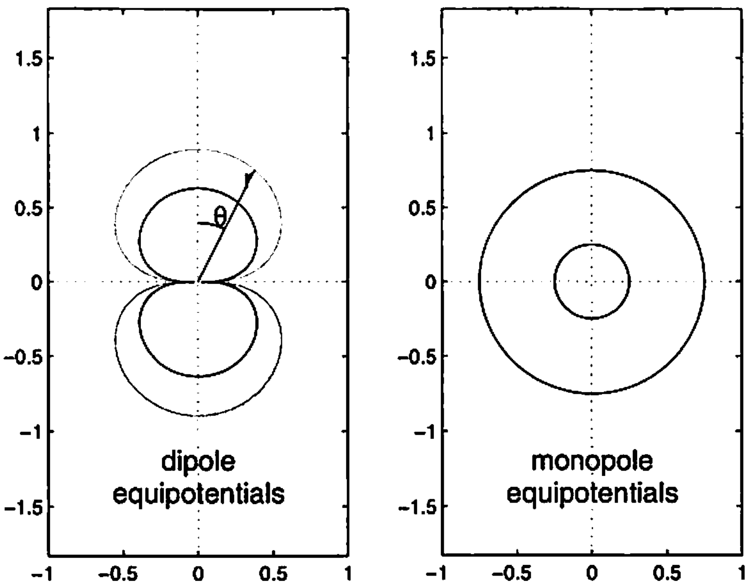

FIGURE 3.12.1. Rotationally symmetric potential as the sum a dipole potential $\left(\mu\frac{\cos\theta}{r^2}\right)$ plus a monopole potential $\left(-\frac{k}{r}\right)$.

$$-\frac{\partial S}{\partial t}=\frac{1}{2m}g^{ij}\frac{\partial S}{\partial x^i}\frac{\partial S}{\partial x^j}+U$$

in terms of the inverse metric.

3.12.2. Separation of Variables. The most important way of solving the H-J equation is by the method of sep[aration of variables. To illustrate this, consider the following

Example (Particle in a dipole potential). Consider the motion of a particle in the potential of a combined dipole and monopole field. Relative to spherical coordinates the metric is

$$(ds)^2=dr^2+r^2d\theta^2+r^2\sin^2\theta\,d\phi^2$$

and that potential has the form

$$U(r,\theta)=\mu\frac{\cos\theta}{r^2}-\frac{k}{r}$$

Its equipotential surfaces are rotationally symmetric around the z-axis

The Lagrangian is

$$
\begin{aligned}
L &= \text{Kinetic Energy } - \text{Potential Energy} \\
&= \frac{1}{2} m\, g_{ij} \dot{q}^i \dot{q}^j - U(q^1, q^2, q^3) \\
&= \frac{1}{2} m\,(\dot{r}^2 + r^2\dot{\theta}^2 + r^2 \sin^2\theta \dot{\phi}^2) - \mu \frac{\cos\theta}{r^2} + \frac{k}{r}\,.
\end{aligned}
$$

The corresponding Hamilto-Jacobi equation is

$$
\begin{aligned}
0 &= \frac{\partial S}{\partial t} + H \\
&= \frac{\partial S}{\partial t} + \frac{1}{2m} g^{ij} \frac{\partial S}{\partial q^i}\frac{\partial S}{\partial q^j} + U(q^1, q^2, q^3) \\
&= \frac{\partial S}{\partial t} + \frac{1}{2m}\left[\left(\frac{\partial S}{\partial r}\right)^2 + \frac{1}{r^2}\left(\frac{\partial S}{\partial \theta}\right)^2 + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial S}{\partial \phi}\right)^2\right] + \mu\frac{\cos\theta}{r^2} - \frac{k}{r}\,.
\end{aligned}
$$

This equation can be solved by the method of separation of variables. This method is condensed into the following three definitions and propositions:

(1) *Definition (Separable variables).* The variables $q^1, q^2, \cdots, q^s$ in the H-J equation

$$0 = \frac{\partial S}{\partial t} + H\left(t, q^i, \frac{\partial S}{\partial q^j}\right) \equiv \mathcal{H}\left(t, \frac{\partial S}{\partial t}, q^i, \frac{\partial S}{\partial q^j}\right)$$

are said to be ***separable*** if it has a "complete" solution of the form

$$S = S_0(t, \alpha_0) + S_1(q^1, \alpha_0, \alpha_1) + S_2(q^2, \alpha_0, \alpha_1, \alpha_2) + S_3(q^3, \alpha_0, \alpha_1, \alpha_2, \alpha_3) \tag{3.12.2}$$

where each S_i depends only on t and q^i respectively.

(2) *Definition (Complete solution).* A solution is said to be ***complete*** if

$$\det\left|\frac{\partial^2 S}{\partial\alpha_i \partial q^j}\right| \neq 0$$

Remark 1: We saw (in Lecture 13) in the context of reconstructing the classical trajectories of a Hamiltonian system from the principle of constructive interference it was essential that the matrix $\left[\partial^2 S/\partial\alpha_i\partial q^j\right]$ be non-singular.

Remark 2: The solution, Eq.(3.12.2), is complete indeed, because

$$
\det\left|\frac{\partial^2 S}{\partial\alpha_i\partial q^j}\right| = \det
\begin{array}{c}
\begin{array}{ccc} 1 & 2 & 3 \end{array} \\
\left|\begin{array}{ccc} * & 0 & 0 \\ * & * & 0 \\ * & * & * \end{array}\right|
\end{array}
\neq 0
\quad
\begin{array}{c} \leftarrow \; j \\ 0 \\ 1 \\ 2 \\ \uparrow \\ i \end{array}
$$

and its diagonal elements are not zero.

(3) *Definition (separability condition).* The Hamilton-Jacobi equation is said to satisfy the separability criterion if its Hamiltonianis is of the form

$$\mathcal{H}\left(t, \frac{\partial S}{\partial t}, q^i, \frac{\partial S}{\partial q^j}\right) = f_3\left(f_2\left(f_1\left(f_0\left(t, \frac{\partial S}{\partial t}\right), q_1, \frac{\partial S}{\partial q^1}\right), q^2, \frac{\partial S}{\partial q^2}\right), q^3, \frac{\partial S}{\partial q^3}\right)$$

(for $s = 3$ degrees of freedom). This functional form is said satisfy the condition of separability because the solution to this first order p.d.e. has the separated form, Eq.(3.12.2). In other words, the claim is

Proposition: Definition 3 implies Definition 1.

Proof: Step 1.) According to Definition 3 the H-J equation is

$$f_3\left(f_2\left(f_1\left(f_0\left(t, \frac{\partial S}{\partial t}\right), q_1, \frac{\partial S}{\partial q^1}\right), q^2, \frac{\partial S}{\partial q^2}\right), q^3, \frac{\partial S}{\partial q^3}\right) = 0\,. \tag{3.12.3}$$

The method of solution via separation of variables starts by solving for f_0. One finds

$$f_0\left(t, \frac{\partial S}{\partial t}\right) = \text{an expression involving } q^1, q^2, q^3, \frac{\partial S}{\partial q^1}, \frac{\partial S}{\partial q^2}, \text{and } \frac{\partial S}{\partial q^3}\,.$$

Assume the solution to have the form

$$S = T(t) + S'(q^1, q^2, q^3)\,. \tag{3.12.4}$$

This assumption is the first step towards success because the resulting common value of

$$\underbrace{f_0\left(t, \frac{dT(t)}{dt}\right)}_{\substack{\text{independent} \\ \text{of } q^1, q^2, q^3}} = \underbrace{\text{an expression that depends only on } q^1, q^2, q^3}_{\text{independent of t}}$$

is independent of all variables. This common independence implies that f_0 is a constant, say, α_0:

$$f_0\left(t, \frac{dT(t)}{dt}\right) = \alpha_0\,.$$

Solving for $T(t)$, one obtains

$$T(t) = S_0(t, \alpha_0)\,. \tag{3.12.5}$$

Step 2.) Using this function in Eq.(3.12.4) and introduce S into Eq.(3.12.3), which now becomes

$$f_3\left(f_2\left(f_1\left(\alpha_0, q^1, \frac{\partial S'}{\partial q^1}\right), q^2, \frac{\partial S'}{\partial q^2}\right), q^3, \frac{\partial S'}{\partial q^3}\right) = 0\,.$$

Solving for f_1 one finds

$$f_1\left(\alpha_0, q^1, \frac{\partial S'}{\partial q^1}\right) = \text{an expression involving } q^2, q^3, \frac{\partial S'}{\partial q^2}, \text{and } \frac{\partial S'}{\partial q^3}\,.$$

Let

$$S' = Q_1(q^1) + S''(q^2, q^3)\,.$$

Consequently,

$$\underbrace{f_1\left(\alpha_0, q^1, \frac{dQ_1(q^1)}{dq^1}\right)}_{\substack{\text{independent} \\ \text{of } q^2, q^3}} = \underbrace{\text{an expression that depends only on } q^2, q^3}_{\text{independent of } q^1}\,.$$

This common independence implies that f_1 is a constant, say, α_1:

$$f_1\left(\alpha_0, q^1, \frac{dQ_1(q^1)}{dq^1}\right) = \alpha_1 .$$

Solving for $Q_1(q^1)$, one obtains

$$Q_1(q^1) = S_1(q^1, \alpha_1) . \tag{3.12.6}$$

Consequently, the solution, Eq.(3.12.4), to the H-J equation has the form

$$S = T(t) + Q_1(q^1) + S''(q^2, q^3) .$$

Step 3.) Repeat Step 2.) two more times to obtain

$$f_2\left(\alpha_0, \alpha_1, q^2, \frac{dQ_2(q^2)}{dq^2}\right) = \alpha_2$$

$$f_3\left(\alpha_0, \alpha_1, \alpha_2, q^3, \frac{dQ_3(q^3)}{dq^{23}}\right) = \alpha_3 .$$

Notice, however, that the H-J Eq.(3.12.3) implies that $\alpha_3 = 0$, always. Consequently, there are only *three* independent separation constants, $(\alpha_0, \alpha_1, \alpha_2)$, while the number of independent variables, (t, q^1, q^2, q^3) , is four. It follows that

$$S = T(t) + Q_1(q^1) + Q_2(q^2) + Q_3(q^3)$$

and hence wth Eqs.(3.12.5), (3.12.6), etc.

$$= S_0(t, \alpha_0) + S_1(t, q^1, \alpha_0, \alpha_1) + S_2(t, q^2, \alpha_0, \alpha_1, \alpha_2) + S_3(t, q^3, \alpha_0, \alpha_1, \alpha_2, \alpha_3 = 0) .$$

Thus the dynamical phase S has indeed the separated form whenever its H-J equation has the form (3.12.3)