SECTION A : BASICS

At present all our formulations of quantum mechanics start from classical mechanics, even when the final result is non-classical. This is true both for particle mechanics (relativistic or not) and for field theory (relativistic or not). Because of this, one needs to go through a somewhat contorted development, via wave-functions (functions defined in Hilbert space), measurements and operator calculus, density matrices & expectation values, before arriving at the underlying physics. Many features of this physics are still being uncovered: basic aspects of quantum mechanics such as entanglement, non-locality, topological phase, and decoherence have only recently become the focus of research, and serve to emphasize how mysterious quantum mechanics still remains.

It is inevitable that at some future time a new formulation will be found which solves some of the paradoxes of Q.M. It is likely that this formulation will not rely on classical mechanics. However we do not yet have this - so in what follows we begin by quickly reviewing important features of classical theory, formulated in terms of Lagrangian & Hamiltonian mechanics. We then recall the formulation of QM. in terms of state vectors in Hilbert space, and the more general (& perhaps fundamental) formulation in terms of density matrices. Then the link to the world around us is made, in terms of quantum measurements, & their association with operators. This gives us our first taste of a fundamental (& non-classical) property of quantum systems, viz., "entanglement". Finally, a quite different formulation of QM is introduced, in terms of "path integrals".

A.1. CLASSICAL MECHANICS

Classical Mechanics deals with the dynamics of both particles & fields. The first formulation of this was given in terms of equations of motion. Modern formulations rely on the existance of an action function for a given set of physical systems, starting from which either a Lagrangian or a Hamiltonian can be extracted, and from which the equations of motion can be derived.

The classical mechanics of particles and solid bodies begins with an idealisation, that of an isolated or quasi-isolated physical system, composed of point particles. A "point particle" is a system in which internal structure or dynamics can be ignored; and according to observation, its physical state can then be entirely characterised by its position and velocity at time t. An isolated physical system (sometimes called a "closed system") is one for which the behaviour (described by the motion in time of of the positions and velocities of the particles in the system) is independent of the behaviour of any other system (ie., of the rest of the universe).

To describe systems of point particles like this one introduces a set of generalised coordinates. We consider 2 systems S_A and S_B, composed of N_A and N_B particles respectively, and define generalised coordinates $Q_A, \dot{Q}_A$, and $Q_B, \dot{Q}_B$, both functions of t. Assuming space is 3-dimensional, we have

$$\left.\begin{aligned} Q_A(t) &= (q_1^A(t), q_2^A(t), \ldots q_{3N_A}^A(t)) & \dot{Q}_A(t) &= (\dot{q}_1^A(t), \ldots \dot{q}_{3N_A}^A(t)) \\ Q_B(t) &= (q_1^B(t), q_2^B(t), \ldots q_{3N_B}^B(t)) & \dot{Q}_B(t) &= (\dot{q}_1^B(t), \ldots \dot{q}_{3N_B}^B(t)) \end{aligned}\right\} \quad (1)$$

A.1.1. ACTION FUNCTIONAL OF L

The behaviour of the generalized coordinates $Q, \dot{Q}$ as functions of time is described by 3 different mathematical frameworks, all of which are equivalent in classical mechanics. All of these are important generalizations of the original formulation by Newton.

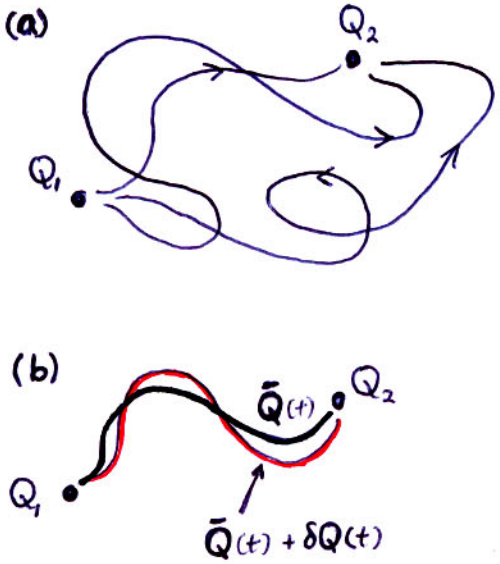
A.1.1(a) LAGRANGIAN, & PRINCIPLE of LEAST ACTION : It is assumed that the system can be described by a single function $L(Q, \dot{Q}; t)$, from which we can also derive the dynamics - this is in line with the above remarks. As we will discuss below, the form of $L(Q, \dot{Q}; t)$ can be deduced at least in part by considering the symmetries inherent in the physical system being discussed.

As a result of work by Euler, Lagrange, and Hamiltonian, a rather remarkable & beautiful derivation of the equations of motion satisfied by any classical system of particles can be given, starting from the Principle of Least Action.

One defines the "Action Functional" $S(Q_2, Q_1; t_2, t_1)$ as follows:

$$S\{Q_2, Q_1; t_2, t_1\} = \int_{t_1}^{t_2} dt\, L(Q(t), \dot{Q}(t); t) \Big|_{\substack{Q(t_2) = Q_2 \\ Q(t_1) = Q_1}} \tag{2}$$

This is a functional over the path $Q(t)$ followed by the system between the times t_1 and t_2, with the constraint that the system begin at position Q_1 and finish at position Q_2. Notice there is no condition on the initial & final velocities, which are arbitrary. Thus S is a complicated functional, since a huge variety of paths (in $3N$-dimensional space) is possible.



(a) PATHS BETWEEN Q_1 AND Q_2

(b) VARIATION OF PATHS AROUND THE PATH $\bar{Q}(t)$.

The actual path followed by the system is specified using the principle of least action, which states that this path $\bar{Q}(t)$ is the one for which $S(Q_2, Q_1; t)$ is a MINIMUM. This leads to a standard variational problem, of the type first studied by Euler. One has

$$\left.\begin{aligned} \delta S(Q = \bar{Q}) &= 0 \\ S(Q = \bar{Q}) &= \min S(Q, \dot{Q}; t) \end{aligned}\right\} \tag{3}$$

where the first condition tells us that the action is an extremum when $Q(t) \to \bar{Q}(t)$, and the 2nd tells us that it is minimized. As is always the case, variation of S around the minimum yields a set of differential equations; we have

$$\left.\begin{aligned} \delta S\{Q, \dot{Q}\} &= \delta\left[\int_{t_1}^{t_2} dt\, L(Q, \dot{Q}; t)\right] = 0 \\ \text{with} \quad \delta Q(t_1) &= \delta Q(t_2) = 0 \end{aligned}\right\} \tag{4}$$

Writing small variations of the path $Q(t)$ around $\bar{Q}(t)$ as $\delta Q(t)$ (with a corresponding variation $\delta\dot{Q}(t)$ in the velocity) we have

$$\left.\begin{aligned} \delta S &= \int_{t_1}^{t_2} dt \left[L(\bar{Q}+\delta Q, \dot{\bar{Q}}+\delta\dot{Q}; t) - L(\bar{Q}, \dot{\bar{Q}}; t) \right] \\ &= \int_{t_1}^{t_2} dt \left[\left.\frac{\partial L}{\partial Q}\right|_{Q=\bar{Q}} \delta Q + \left.\frac{\partial L}{\partial \dot{Q}}\right|_{\dot{Q}=\dot{\bar{Q}}} \delta\dot{Q} \right] = 0 \end{aligned}\right\} \quad (5)$$

One integrates the 2nd term by parts to get everything in terms of δQ, viz:

$$\left.\begin{aligned} \int_{t_1}^{t_2} dt \, \frac{\partial L}{\partial \dot{Q}} \delta\dot{Q} &= \left[\frac{\partial L}{\partial \dot{Q}} \delta Q \right]_{t_1}^{t_2} - \int_{t_1}^{t_2} dt \, \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{Q}}\right) \delta Q \\ &= - \int_{t_1}^{t_2} dt \, \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{Q}}\right) \delta Q \end{aligned}\right\} \quad (6)$$

where the 1st term on the R.H.S. is zero because $\delta Q(t_1) = \delta Q(t_2) = 0$ (cf (4)). Thus we have

$$\delta S = \int_{t_1}^{t_2} dt \left(\frac{\partial L}{\partial Q} - \frac{d}{dt}\frac{\partial L}{\partial \dot{Q}} \right) \delta Q \quad (7)$$

and because $\delta Q(t)$ is arbitrary, we immediately get the Euler-Lagrange eqns:

$$\boxed{\begin{aligned} &\frac{d}{dt}\frac{\partial L}{\partial \dot{Q}} - \frac{\partial L}{\partial Q} = 0 \\ \text{ie} \quad &\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0 \qquad \forall\, j = 1,2,3,\ldots 3N \end{aligned}} \quad (8)$$

These equations reduce to those of Newton under circumstances described below. We have now 2 different formulations of the dynamics of classical point particles, in terms of either an action function, or as a set of differential equations.

A.I.1(b) FORM OF L; SYMMETRIES

: A key feature of classical mechanics, which has been of enormous importance in quantum physics, is the fact that one can deduce some (or sometimes all) the dependence of $L(Q, \dot{Q}; t)$ on $Q, \dot{Q}$, and t, simply by considering the symmetries obeyed by the system. An added benefit of this manoeuvre is that we deduce the conservation laws (constants of the motion) of the physical system.

Because this is not a course in classical mechanics, I only summarize the main results here, with brief notes on their derivation. They can be given in tabular form:

(i) Independent Systems : By definition, these are systems for which the equations of motion of one is not affected by the other. This implies that

$$\boxed{L = L_A^\circ + L_B^\circ} \tag{9}$$

for 2 independent systems A and B; here $L_A^\circ = L_A^\circ(Q_A, \dot{Q}_A; t)$ and likewise $L_B^\circ = L_B^\circ(Q_B, \dot{Q}_B; t)$ (cf eqtn (1)).

Note that we are free to multiply L_B° and L_A° by arbitrary constants, but these must be the same constants if we want consistency if the systems ever do interact with each other.

(ii) Addition of Total Time derivative : We are free to add to a given L a function $f(Q,t)$ which is a total time derivative, ie, if $L(Q,\dot{Q};t)$ is a correct Lagrangian for some system, then so is $L'(Q,\dot{Q}';t)$, where

$$\boxed{\begin{aligned} L' &= L + \frac{d}{dt} f(Q,t) \\ S' &= S + (f_2 - f_1) \end{aligned}} \tag{10}$$

It is easy to see that such a shift makes no difference to the equations of motion or to the minimization of S.

(iii) Homogeneity of Space (Galilean Invariance) : If a system is closed, ie., independent of any other system, then its dynamics must be independent of its position. It then follows that L is independent of Q, ie.

$$L(Q,\dot{Q};t) \rightarrow L_0(\dot{Q},t) \tag{11}$$

and from this one derives the CONSERVATION of MOMENTUM; defining $P = \partial L/\partial \dot{Q}$, we have

$$\boxed{\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{Q}}\right) = \dot{P} = 0} \quad \text{(closed system)} \tag{12}$$

(iv) Homogeneity of Time : For a closed system, there is also no preferred time (since this would imply an external influence). Thus we have

$$L(Q,\dot{Q};t) \rightarrow L_0(Q,\dot{Q}) \tag{13}$$

and from this one can deduce the CONSERVATION of ENERGY : define $E = \dot{Q}\frac{\partial L}{\partial \dot{Q}} - L$, we have

$$\boxed{\frac{dE}{dt} = \frac{d}{dt}\left[\dot{Q}\frac{\partial L}{\partial \dot{Q}} - L\right] = 0} \quad \text{(closed system)} \tag{14}$$

a result which is easily derived by noting that (13) implies that $\partial L/\partial t = 0$, and showing that $\partial L/\partial t = \frac{d}{dt}[\dot{Q}\,\partial L/\partial \dot{Q}]$.

(v) Isotropy of Space (Rotational Invariance) : Again, if we have a closed system, then there can be no "force" which singles out any orientation for it. If we define this orientation by an angular vector, then this implies that any infinitesimal rotation leaves L invariant, ie

$$\boxed{\frac{\partial L}{\partial \underline{\phi}} = 0} \qquad (15)$$

where $\delta\underline{\phi}$ is the infinitesimal rotation, in 3d space.

(vi) Influence of Interactions : Suppose we have a closed system S which we then divide into 2 parts, which we call system A and system B. The above remarks apply to S, but not to S_A and S_B individually. Nevertheless in NON-RELATIVISTIC classical mechanics we can make a fairly stringent requirement on the form of the Lagrangian. In fact spacetime homogeneity implies that the total Lagrangian must have the form

$$\boxed{L_S(Q_A, Q_B; \dot{Q}_A, \dot{Q}_B) = L_A^0(Q_A, \dot{Q}_A) + L_B^0(Q_B, \dot{Q}_B) + L_{int}(Q_A, Q_B)} \qquad (16)$$

so that there is an additive interaction, which is a function only of the coordinates of the 2 systems, and not their velocities. The latter feature implies that the interactions described by L_{int} are propagating instantaneously - any dependence on velocities would violate spacetime homogeneity of these interactions. The interaction terms must be additive because otherwise it would not separate from L_B^0 and L_B^0 (the same kind of argument that gave (9)). By convention one writes

$$V_{int}(Q_A, Q_B) = - L_{int}(Q_A, Q_B) \qquad (17)$$

thereby defining the potential energy function $V_{int}(Q_A, Q_B)$. Note that the isotropy of space also implies that $V_{int}(Q_A, Q_B)$ must be a function of $|Q_A - Q_B|$, ie of $|\underline{r}_i^A - \underline{r}_j^B|$, where $\underline{r}_i^A$ is the coordinate of a particle in system A and $\underline{r}_j^B$ the coordinate of a particle in system B.

It is useful to rewrite all these results for a set of N interacting particles, in which there exists an interaction $V_{int}(\underline{r}_1, \underline{r}_2, \ldots \underline{r}_N)$ between the particles. The Lagrangian for the total system then reads

$$\boxed{\begin{aligned} L(Q, \dot{Q}) &= T - V \\ T &= L_0(\dot{Q}) \equiv L_0(\dot{\underline{r}}_1, \dot{\underline{r}}_2, \ldots \dot{\underline{r}}_N) = \sum_{j=1}^{N} L_0^j(\dot{\underline{r}}_j) \\ V &= V_{int}(\underline{r}_1, \underline{r}_2, \ldots \underline{r}_N) \end{aligned}} \qquad (18)$$

where $T = \sum_j T_j(\dot{\underline{r}}_j)$ is the kinetic energy, and V the potential energy. The kinetic energy is a function of $\dot{Q}$ only, because of (11) and (13), and is again additive. The general form is

$$T = \sum_j T_j = \frac{1}{2} \sum_j m_j \dot{\underline{r}}_j^2 \qquad (19)$$

To derive (19) one argues as follows. Isotropy implies that T_j must be a function of $|\dot{r}_j|^2$; a term like $|\dot{r}_j|$ is ruled out because it would lead to pathological behaviour at $|\dot{r}_j| = 0$. To show it is a linear function of $\dot{Q}^2$, we can compare 2 reference frames R and R', shifted from each other by an infinitesimal velocity $\delta \underline{V}$. Then the Lagrangians in the 2 frames are related by

$$L_0'(\dot{r}_j) = T'(\dot{r}_j) - T(\dot{r}_j) + \frac{\partial T}{\partial \dot{r}_j} \cdot \delta \underline{V} \qquad (20)$$

and from (10) we have $$\frac{\partial T}{\partial \dot{r}_j} \cdot \delta \underline{V} = \frac{d}{dt} f(r_j; t) \qquad (21)$$

$$\text{so that} \quad f(r_j; t) = \delta \underline{V} \cdot \int dt \, \partial T / \partial \dot{r}_j$$

For $f(r_j; t)$ to be independent of $\dot{r}_j$, $T(\dot{r}_j)$ must be proportional to $\dot{r}_j^2$; any other functional behaviour would give a dependence on $\dot{r}_j$ in f.

The conservation laws now take the form:

$$\boxed{\begin{aligned} \dot{\underline{P}} &= \sum_j \dot{\underline{p}}_j = \frac{d}{dt} \sum_j m_j \dot{r}_j \\ \frac{dE}{dt} &= \frac{d}{dt}\left[\sum_j \dot{r}_j \cdot \frac{\partial T_j}{\partial \dot{r}_j} - L \right] = \frac{d}{dt}(T+V) = 0 \\ \frac{d\underline{L}}{dt} &= \frac{d}{dt}\left(\sum_j r_j \times p_j \right) = \frac{d}{dt} \sum_j \underline{l}_j = 0 \end{aligned}} \qquad (22)$$

The proof that (15) implies the conservation of angular momentum $\underline{L}$ is left as an exercise.

Finally, notice that in classical non-relativistic mechanics we can always write the influence of another system on a given system in terms of a time-dependent force. Starting from (16), we notice that we can write the dynamics of S_A entirely in terms of a Lagrangian

$$\left.\begin{aligned} L_A &= T(\dot{Q}_A) - U(Q_A, Q_B(t)) \\ U(Q_A, Q_B) &= V_A(Q_A) + V_{int}(Q_A, Q_B(t)) \end{aligned}\right\} \qquad (23)$$

where the dynamics of the external coordinate is assumed to be known - it is this coordinate $Q_B(t)$ that gives the potential V_{int} its time dependence. Note however that in general we cannot find $Q_B(t)$ without solving the complete coupled dynamics of $S = S_A + S_B$; this result is only useful if the back-reaction of S_A on S_B is negligible.

THE EQUIVALENCE, FOR SYSTEM A, OF THE EXTERNAL INTERACTION U TO THE INTERACTION V_{int} WITH SYSTEM B

A.1.2. THE HAMILTONIAN $\mathcal{H}$

In a development that turned out to be crucial for the genesis of Q.M. Hamilton formulated a different derivation of classical mechanics. We define the generalized momentum of the system as

$$P = \partial L / \partial \dot{Q} \tag{24}$$

(as in (12) above), and then rewrite everything in terms of P and Q (instead of Q and $\dot{Q}$). This is easily done using a Legendre transformation - we define the new HAMILTONIAN function

$$\boxed{\mathcal{H}(P,Q;t) = P\dot{Q} - L} \tag{25}$$

and it is then easy to show that

$$d\mathcal{H} = \dot{Q}\,dP - \dot{P}\,dQ \tag{26}$$

from which it follows that

$$\boxed{\begin{aligned} \dot{Q} &= \partial\mathcal{H}/\partial P \\ \dot{P} &= -\partial\mathcal{H}/\partial Q \end{aligned}} \tag{27}$$

otherwise known as Hamilton's eqtns of motion.

We can derive these starting from a different form of the principle of least action. From (25) and (2) we can write that

$$S = \int_{t_1}^{t_2} dt\, [P\dot{Q} - \mathcal{H}(P,Q)] \tag{28}$$

ie

$$\boxed{S \equiv \int P\,dQ - \mathcal{H}\,dt} \tag{29}$$

where the limits on the first integral are just the initial & final positions Q_1 and Q_2. If we now vary this action, we get

$$\left.\begin{aligned} \delta S &= \int [(\delta P\,dQ + P\,d\delta Q] - [\frac{\partial\mathcal{H}}{\partial Q}\delta Q + \frac{\partial\mathcal{H}}{\partial P}\delta P]\,dt \\ &= \int [dQ - \frac{\partial\mathcal{H}}{\partial P}dt]\,\delta P - \int [dP + \frac{\partial\mathcal{H}}{\partial Q}dt]\,\delta Q \end{aligned}\right\} \tag{30}$$

where we drop the total integral $[P\,dQ]$ because $\delta Q = 0$ at the limit points. Normally one writes (30) as

$$\delta S = \int dt \left\{ [\dot{Q} - \frac{\partial\mathcal{H}}{\partial P}]\,\delta P - [\dot{P} + \frac{\partial\mathcal{H}}{\partial Q}]\,\delta Q \right\} \tag{31}$$

but one sees immediately from either (29) or (30) that on the extremal path, when $\delta S = 0$, both the variations in δP and δQ must vanish, and we again recover Hamilton's eqtns.

The interesting thing is that at first glance we appear to have transformed the $3N$ independent eqtns of motion in (8) to a new set of $6N$ independent eqtns of motion in (27). This is of course impossible, and we resolve this paradox below.

A.1.2(a) CANONICAL TRANSFORMATIONS:

Hamilton's eqtns make no real distinction between the variables P and Q, and so one may easily imagine coordinate transformations of the form

$$Q \to Q'(P,Q;t) \qquad P \to P'(P,Q;t)$$
$$\mathcal{H} \to \mathcal{H}'(P',Q';t) \qquad (32)$$

However the new variables must also obey Hamilton's eqtns, ie., we require

$$\dot{Q}' = \partial\mathcal{H}'/\partial P' \qquad \dot{P}' = -\partial\mathcal{H}'/\partial Q'$$
$$\text{and} \quad \delta S' = \delta\int[P'dQ' - \mathcal{H}'dt] = 0 \qquad (33)$$

Comparing (29) and (33) we see that S and S' can only differ by the total differential dF of a function $F(Q,Q';t)$, ie

$$(P'dQ' - \mathcal{H}'dt) - (P\,dQ - \mathcal{H}\,dt) = dF \qquad (34)$$

where we see that $F = F(Q,Q';t)$ because Q, Q', t have differentials in (34). The function $F(Q,Q';t)$ is the generating function of the transformation, with results

$$P = -\partial F/\partial Q \qquad P' = \partial F/\partial Q' \qquad \mathcal{H}' = \mathcal{H} - \partial F/\partial t \qquad (35)$$

Now there is nothing inevitable about using a transformation which is a function of Q, Q', and t; one can use any one of the combinations Q,Q', or Q,P', or P,Q', or P,P'. Consider, eg., a generating function $G(Q,P';t)$; to implement this we need to first make a Legendre transformation on the function $F(Q,Q';t)$ to convert the free variables from Q,Q' to Q,P'. Defining

$$G(Q,P';t) = P'Q' - F(Q,Q';t) \qquad (36)$$

we have
$$dG = (P\,dQ + Q'\,dP') + (\mathcal{H}' - \mathcal{H})\,dt$$
and
$$P = \partial G/\partial Q \qquad Q' = \partial G/\partial P' \qquad \mathcal{H}' = \mathcal{H} + \partial G/\partial t \qquad (37)$$

Let us note 3 interesting implications of this in passing. Notice first that among the many possible canonical transformations, the simplest one is produced by simply swapping the roles of P and Q. This can be done using a generating function $F(Q,P') = QP'$, to produce $P \to Q'$, $Q \to -P'$. Thus there is nothing fundamental in the distinction between momentum and position coordinates.

The second remark is concerning the use of time-dependent canonical transformations - it is obvious from (35) and (37) that this shifts $\mathcal{H}$ ($\mathcal{H}'$ and $\mathcal{H}$ are the same otherwise), in general to a time-dependent form. This can be very useful if, eg., one wants to go to some moving frame of reference.

Third, notice that one interesting canonical transformation is generated by the action S itself. For let $P(t+\delta t) = P'$, and $Q(t+\delta t) = Q'$ (and if $\mathcal{H}$ depends on time, $\mathcal{H}(t+\delta t) = \mathcal{H}'$. Then the change δS between the two times is just

$$\delta S = (P'dQ' - P\,dQ) - (\mathcal{H}' - \mathcal{H})\,dt \qquad (38)$$

using (29) and (33); comparing with (34), we get the required result.

Canonical transformations turn out to be a powerful tool in both classical and quantum mechanics, as we will see.

A.1.2(b) HAMILTONIAN FLOW in PHASE SPACE

: Normally one thinks of the dynamics of a set of N particles in terms of a point moving in $3N$-dimensional space with coordinate Q and velocity $\dot{Q}$. In the Hamiltonian description one expands this to the dynamics of a particle in $6N$-dimensional <u>phase space</u>. Of course the number of degrees of freedom has not changed - it is $6N$ in both cases. However the way the system "flows" in phase space is very interesting.

Let's begin by defining a "fluid" in this space, by a set of $\mathcal{N}$ "particles", each representing a particular system. We have thus chosen an ensemble of systems, and lets assume some initial distribution $\rho(P,Q)$ of these particles in the phase space. (ie., ρ is a density in phase space for this ensemble)

Now the assumption that $\mathcal{N}$ is conserved means that

$$\frac{\partial}{\partial t}\rho + \nabla_{PQ}\cdot(\rho \underline{v}) = 0 \qquad \text{(conservation of } \mathcal{N}\text{)} \tag{39}$$

where we define the "velocity" in phase space by

$$\underline{v} = (\dot{P}, \dot{Q}) \equiv (\dot{P}_1, \dot{P}_2, \ldots \dot{P}_{3N}; \dot{q}_1, \dot{q}_2, \ldots \dot{q}_{3N}) \tag{40}$$

and the gradient operator is

$$\left.\begin{aligned} \nabla_{PQ} &\equiv \hat{P}\,\partial/\partial P + \hat{Q}\,\partial/\partial Q \\ &\equiv \left[\hat{P}_1\,\partial/\partial p_1 + \hat{P}_2\,\partial/\partial p_2 + \cdots + \hat{q}_{3N}\,\partial/\partial q_{3N}\right] \end{aligned}\right\} \tag{41}$$

where $\hat{P}_j, \hat{q}_j$ are unit vectors.

Now Hamilton's eqns imply that the flow in phase space is actually incompressible, ie., that $d\rho/dt = 0$. To show this, we start from (39) and expand it out:

$$\partial_t\rho + \nabla_{PQ}\cdot(\rho\underline{v}) = \partial_t\rho + \rho\left(\frac{\partial\dot{Q}}{\partial Q} + \frac{\partial\dot{P}}{\partial P}\right) + \dot{Q}\left(\frac{\partial\rho}{\partial Q}\right) + \dot{P}\left(\frac{\partial\rho}{\partial P}\right) = 0 \tag{42}$$

However Hamilton's eqns (27) imply that the 2nd term is zero:

$$\partial\dot{Q}/\partial Q + \partial\dot{P}/\partial P = \frac{\partial^2 H}{\partial Q\partial P} - \frac{\partial^2 H}{\partial P\partial Q} = 0 \tag{43}$$

and so

$$\boxed{\frac{d\rho}{dt} = \left[\partial_t + (\dot{P}\partial_P + \dot{Q}\partial_Q)\right]\rho = 0} \tag{44}$$

This fundamental result is known as LIOUVILLE'S THEOREM. The proof given above is elementary. Older texts give a laborious proof in terms of the Jacobian of the time transformation generated by the eqns of motion. Newer texts rewrite everything in terms

of differential forms in phase space. This latter viewpoint has the advantage of being more explicitly geometrical (for details see mathematical appendix M.1).

Let us now look at how some other quantities flow in phase space. Consider any function $f(P,Q)$ defined for some classical system. Then as the system evolves, we have for the change with time of $f(P,Q;t)$:

$$\frac{d}{dt} f(P,Q;t) = \partial_t f + \dot{Q}\frac{\partial f}{\partial Q} + \dot{P}\frac{\partial f}{\partial P} \tag{45}$$

Suppose we introduce the Poisson bracket notation for 2 quantities f and g, both defined in phase space:

$$[f,g] = \frac{\partial f}{\partial P}\frac{\partial g}{\partial Q} - \frac{\partial f}{\partial Q}\frac{\partial g}{\partial P} \tag{46}$$

Then from (45) and from Hamilton's eqns, we immediately have

$$\boxed{\frac{df(P,Q,t)}{dt} = \partial_t f + [H,f]} \tag{47}$$

One of the most interesting quantities to consider in this respect is the action itself. We have

$$\begin{aligned}\frac{dS}{dt} &= \partial_t S + [H,S] \\ &= \partial_t S + \frac{\partial H}{\partial P}\frac{\partial S}{\partial Q} - \frac{\partial H}{\partial Q}\frac{\partial S}{\partial P} \\ &= \partial_t S + \dot{Q}\frac{\partial S}{\partial Q} \\ &= \partial_t S + P\dot{Q}\end{aligned} \tag{48}$$

where we drop the last term in the 2nd line because we know from (29) that dS depends on dQ and dt but not on dP. But we now can immediately infer that

$$\boxed{\begin{aligned}&(a)\quad \frac{\partial S}{\partial Q} = P \\ &(b)\quad \frac{\partial S}{\partial t} = -H(P,Q;t)\end{aligned}} \tag{49}$$

and, from the definition $S = \int L\,dt$, that

$$\boxed{\frac{d}{dt} S = L(Q,\dot{Q};t)} \tag{50}$$

These equations have fundamental significance both in classical & quantum mechanics,

as we will see. To get a handle on what they mean, note that (50) says that if we follow a particle or system along a "streamline" through phase space, staying with it, then the rate of change of S with time is L. But this is made up of 2 changes: one is simply along the trajectory, so that if we "freeze" the system, we see this - this is $\partial S/\partial Q = P$. The other is the pure time dependence, which we would see with some "internal clock" sitting on the particle - this is $\partial_t S = -\mathcal{H}$.

In classical mechanics we see the full significance of this if we look not just at systems of point particles, but also rays in optics, and at fields. In Q.M. it is central to the whole theory. Historically Hamilton formulated his approach in an attempt to put ray optics on the same footing as Newtonian mechanics; and Schrödinger formulated Q.M. as a wave mechanics based on Hamilton's formulation.

HAMILTON-JACOBI EQUATION : By substituting (49a) into (49b), we immediately recover an equation which turns out to be practically quite useful:

$$\boxed{\frac{\partial S}{\partial t} + \mathcal{H}\left(\frac{\partial S}{\partial Q}, Q; t\right) = 0} \tag{51}$$

This is the Hamilton-Jacobi equation, which also gives a useful picture of flow in phase space; it was the link for Schrödinger to his discovery of his famous equation.

We shall not spend long on this equation - just a few select points will be recalled. First, suppose that $\mathcal{H}$ is time-independent (ie., we have a closed system). Then we have

$$\mathcal{H} \to \mathcal{H}_0(Q, \partial S/\partial Q) = E_0 \tag{52}$$

where E is the energy, and we can write

$$\boxed{S = S_0(Q) - E_0 t} \tag{53}$$

Now for such a time-independent closed system one can sometimes make a canonical transformation, first noted by Delaunay, to a set of momenta and coordinates in which the momenta are constants of the motion, and all the time-dependence is in the "positions"; one writes

$$\left.\begin{aligned}(P, Q) \to (P', Q') &\equiv (J, \theta(t)) \\ &\equiv (J_j, \theta_j(t))\end{aligned}\right\} \tag{54}$$

where the new momenta $P' \equiv J$ are called the "action variables", and the new coordinate variables $Q' \equiv \theta$ are called the "angle variables". The generating function for this transformation is of the "G-type" (eqns (36) and (37)), ie., from free variables $P, Q \to Q, P' \equiv Q, J$, and in fact the generating function is $S_0(Q)$ itself, ie

$$G(Q, P') = G(Q, J) = S_0(Q, J) \tag{55}$$

Now it is crucial to understand here that we can <u>only</u> do this if there really

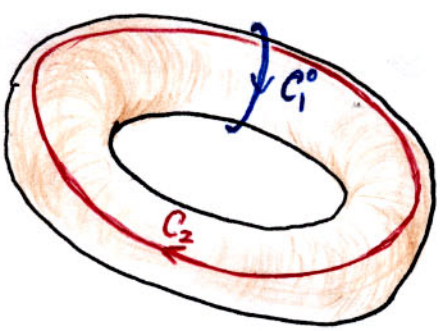
are $3N$ constants of the motion which we can use as the new canonical momenta. To understand under what circumstances such constants do exist for a general classical system is a very difficult problem, which is certainly far from being solved in general. However certain major advances were made in the 20th century on this problem, associated mainly with Poincaré, and Kolmogorov, Arnold, & Moser. A very brief summary of the present situation is as follows:

(a) Integrable Systems: In this case we have $3N$ constants of motion. It can then be shown (most elegantly using methods from topology & differential geometry), that the system must move on a $3N$-dimensional differential manifold in the $6N$-dimensional phase space, which has the topology of a $3N$-dimensional torus. The basic underlying picture is fairly simple - the system has quasi-periodic behaviour, in which there are $3N$ natural frequencies $\{\omega_j^0\}$ to the motion. One can define $3N$ topologically independent paths on the $3N$-torus, none of which can be continuously deformed into any other - how this works for a 2-torus is shown in the Figure at left. There are then $3N$ natural periods of motion of the system, given by (the superscript "0" means 'integrable'):

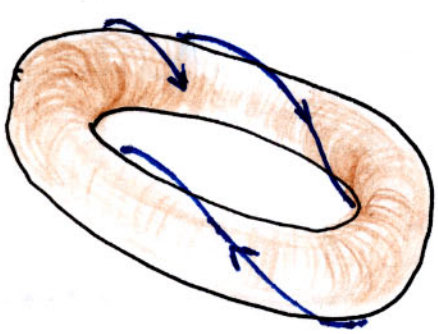
$$T_j^0 = 2\pi/\omega_j^0 \qquad (56)$$

and these are the times taken for the system to make a single circuit of one of the closed path C_j on the $3N$-torus.

(a)



(b)



(a) TWO INDEPENDENT CLOSED CURVES C_1^0 AND C_2^0 ON THE 2-TORUS.

(b) A PATH MADE FROM C_1^0 AND C_2^0, WHICH IS BI-PERIODIC, BUT NOT CLOSED

Of course a much more familiar way of thinking about this is to imagine that one can resolve the dynamics of the system into a Fourier sum of form

$$\left.\begin{aligned} Q(t) &\equiv (q_1(t), q_2(t), \ldots q_{3N}(t)) \\ &= \prod_{j=1}^{3N} \sum_{n_j=-\infty}^{\infty} Q_{n_1 n_2 \ldots n_{3N}} e^{i \sum_j n_j \omega_j^0 t} \end{aligned}\right\} \qquad (57)$$

A Fourier resolution of this motion (or indeed of any other quantity $f(P,Q)$ defined by this motion, which would have a similar expansion

$$f(Q(t)) = \prod_{j=1}^{3N} \sum_{n_j=-\infty}^{\infty} f_{n_1 \ldots n_{3N}} e^{i \sum_j n_j \omega_j^0 t} \qquad (58)$$

would allow one to extract the frequencies and the coefficients. Note, however, that since in general the frequencies $\{\omega_j^0\}$ are incommensurate, ie., not related by any finite fraction, the motion is quasi-periodic, ie, it will never repeat itself in any finite time - this means that a Fourier transform over an infinite time would be required to extract the correct frequencies. Note, however, that as proved by Poincaré, the system will come arbitrarily close to any point on the torus after a finite time, even though paths don't close.

With these preparatory remarks we can now say a little more about

action-angle variables. As understood by Delaunay in 1846, the way to do this was to define the new momenta J_j° in terms of the action accumulated around a single closed curve C_j°, i.e., to write

$$\boxed{J_j^\circ = \frac{1}{2\pi}\oint_{C_j} P\,dQ \equiv \frac{1}{2\pi}\bar{S}_j^{(0)}} \tag{59}$$

Note the accumulated action $\bar{S}_j^{(0)}$ around this curve is just the area in phase space of this curve, and that the canonical transformation can now be written as

$$p_j = \frac{\partial S_0}{\partial q_j} \qquad \theta_j^\circ = \frac{\partial S_0}{\partial J_j^\circ} \tag{60}$$

so that Hamilton's eqtns become

$$\boxed{\begin{aligned} &(a)\quad \dot{J}_j^\circ = -\frac{\partial \mathcal{H}_0}{\partial \theta_j} \longrightarrow 0 \quad (\mathcal{H}_0 \text{ indep. of } t.) \\ &(b)\quad \dot{\theta}_j^\circ = \frac{\partial \mathcal{H}_0}{\partial J_j^\circ} = \omega_j^\circ \end{aligned}} \tag{61}$$

where the frequencies

$$\boxed{\omega_j = \frac{\partial \mathcal{H}_0}{\partial J_j} \equiv \frac{\partial E_0}{\partial J_j}} \tag{62}$$

and $\theta_j(t) = \omega_j t + \alpha_i$, where the $\{\alpha_i\}$ are a set of integration constants. Thus we find the crucial connection between the fundamental frequencies of the system, and the dependence of the energy on the action variables.

Note a further simplification that occurs if the action is separable in the initial set of coordinates Q (or some other appropriate set of initial coordinates. Then we can write

$$\left.\begin{aligned} S_0(\Phi) &\longrightarrow \sum_j S_0^{(j)}(q_j) \\ &= \sum_j J_j^\circ \theta_j^\circ(t) \end{aligned}\right\} \text{(SEPARABLE)} \tag{63}$$

and we can then think of the system as a set of non-interacting oscillators. Note that many important systems are not like this (eg., interacting planetary bodies) and so are hard to deal with even when they are integrable

(b) Non-Integrable Systems

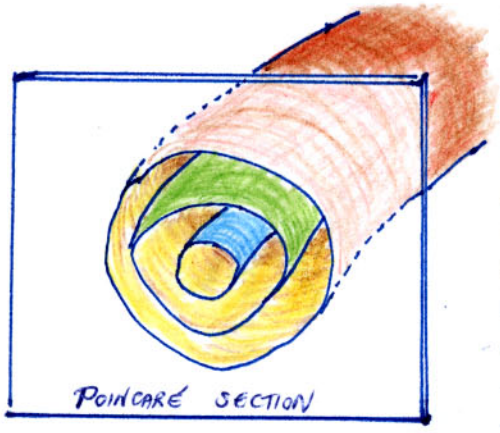
These are much harder to deal with, & I won't say much about them here. We have seen that the motion of integrable systems is confined to "invariant torus" surfaces in phase space - note how little of the phase space is filled by one of these (eg., a single 2-d oscillator torus occupies a tiny part of the vast 4-d phase space in which it lives).

Now suppose we imagine perturbing the system away from some integrable Hamiltonian, and ask the question - what will the motion look like now? This question first began to be

posed in the context of planetary motion, in a serious way by Laplace, 200 yrs ago; it can be formulated in the geometric way we are using here as follows. Suppose we add to the integrable Hamiltonian $\mathcal{H}_0(P,Q) \equiv \mathcal{H}_0(Q,J_0)$ a small perturbation $V(P,Q)$, so that we have

$$\mathcal{H}(P,Q) = \mathcal{H}_0(P,Q) + V(P,Q) \qquad (64)$$

What then happens to the motion on the torus? Usually this question is asked with the dependence of the phase space action integrals J_j^0 on the energy E_0 in mind - as we increase the total energy of the system, the tori expand (cf. eqtn (62)). At a given energy the system moves over the surface of a single torus - its motion can be visualised in various ways, and one simple one is to imagine mapping out the points it passes through when it crosses a "Poincaré section", which is a hyperplane in phase space which cuts through the torus.



INVARIANT TORI OF DIFFERENT ENERGY, INTERSECTING A POINCARÉ SECTION (FLAT HYPERPLANE).

The question then is - what happens to the tori, and to the motion on them, when we add $V(P,Q)$?

This is not a simple question to answer - opinions have varied from "nothing much" (eg., Landau & Lifshitz) to a very rapid destruction of the invariant tori, ie., some very complex motion with no relationship to these tori (the opinion of Poincaré, and also of Fermi & Ulam, at least until they began to do computer simulations).

One obvious manoeuvre, pursued by Laplace & many others, is to use perturbation theory. Suppose we write the perturbation in the same form as (58), viz.,

$$\left.\begin{aligned} V(Q,J;t) &= \prod_{j=1}^{3N} \sum_{n_j=-\infty}^{\infty} V_{n_1 \ldots n_{3N}}(J_1^0, J_2^0 \ldots J_{3N}^0)\, e^{i \sum_j n_j \omega_j^0 t} \\ &\equiv \sum_{\underline{n}} V_{\underline{n}}(J_0)\, e^{i \underline{n}\cdot\underline{\omega}^0 t} \end{aligned}\right\} \qquad (65)$$

where the 2nd form is a condensed notation with vectors in $3N$ dimensional space, and a sum over $\underline{n} = (n_1, n_2 \ldots n_{3N})$ with each n_j varying from $+\infty$ to $-\infty$.

It is then straightforward to verify that to 1st order in V, the invariant tori actions are changed as follows:

$$\left.\begin{aligned} S_0 &\to S_0 + S_1 \\ S_1 &= i \sum_{\underline{n}}{}' \frac{V_{\underline{n}}(J_0)}{\underline{n}\cdot\underline{\omega}^0}\, e^{i \underline{n}\cdot\underline{\omega}^0 t} \end{aligned}\right\} \qquad (66)$$

where the prime on the summation means one omits the $\underline{n} = 0 \equiv (0,0,0 \ldots 0)$ term. Likewise the 1st-order change in the motion is

$$Q(t) \to Q(t) + \delta Q(t) \qquad \delta Q(t) = \int^t dt'\, V(Q,t')\, \Phi(t') \qquad (67)$$

which we evaluate by expanding both V and Q in a Fourier series, to get

$$\left.\begin{aligned} \delta Q(t) &\sim \int^t dt' \sum_{\underline{n}\underline{m}} V_{\underline{n}} Q_{\underline{m}} e^{i(\underline{n}+\underline{m})\cdot\underline{\omega}^0 t'} \\ &\sim \sum_{\underline{n}\underline{m}} \frac{V_{\underline{n}} Q_{\underline{m}}}{(\underline{n}+\underline{m})\cdot\underline{\omega}^0} e^{i(\underline{n}+\underline{m})\cdot\underline{\omega}^0 t} \end{aligned}\right\} \quad (68)$$

now the trouble with expressions like (66) and (68) is that the energy denominators can become very small or even zero - expanding them out, we have

$$\left.\begin{aligned} \sum \underline{n}\cdot\underline{\omega}_0 &\equiv \sum_{n_j=-\infty}^{\infty} n_j \omega_j^0 \equiv n_1\omega_1^0 + n_2\omega_2^0 \ldots n_{3N}\omega_{3N}^0 \\ \sum (\underline{n}+\underline{m})\cdot\underline{\omega}_0 &\equiv \sum_{n_j=-\infty}^{\infty} \sum_{m_k=-\infty}^{\infty} (n_j\omega_j^0 + m_k\omega_k^0) = \text{etc.} \end{aligned}\right\} \quad (69)$$

If any 2 frequencies ω_i^0 and ω_j^0 are commensurate then by letting $n_i/n_j = -\omega_j^0/\omega_i^0$, we get $n_i\omega_i^0 + n_j\omega_j^0 = 0$. Even if no two frequencies are commensurate, we can make the sum $n_i\omega_i^0 + n_j\omega_j^0$ as small as we want by using close values of n_i/n_j which closely approximate the ratio $-\omega_j/\omega_i$. It is a well-known result of number theory that if one uses values of $|n_i|, |n_j| \sim O(M)$, then the difference $|\omega_i/\omega_j| - |n_i/n_j| \sim O(M^{-2})$, so that we can again make the denominator arbitrarily small.

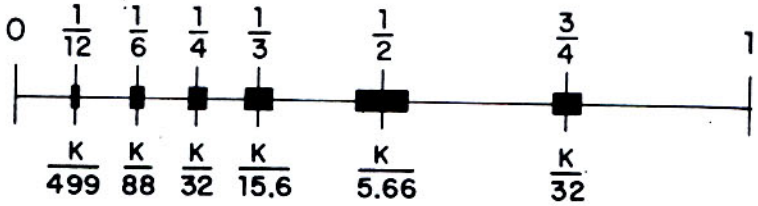
Thus perturbation theory breaks down completely, and for 150 yrs the question of how generic integrable behaviour was, & what happened away from it, was unsolved (as were related problems about the stability of mechanical systems like the solar system). There was certainly no doubt that the resonant interactions occuring when energy denominators were small were physically real, and had important long-time effects - but what ultimately happened?

The problem was solved by the famous "KAM theorem" (Kolmogorov, 1954; Arnold, Moser, 1962). Here is one statement of it:

"If $|V|$ is sufficiently small, then for almost all irrational $\underline{\omega}^0$ there exists an invariant Torus $T_1(\underline{\omega}^0)$ of the perturbed system such that $T_1(\underline{\omega}^0)$ is close to the unperturbed torus $T_0(\underline{\omega}^0)$"

The meaning of this is roughly the following. If the unperturbed system has a rational $\underline{\omega}^0$ (ie, if there are commensurate frequencies ω_i^0, ω_j^0), then an arbitrarily small perturbation will destroy T_0. However if ω^0 is irrational, then this is not the case - a sufficiently small V will not destroy the invariant Torus structure. Now the key point is this - although the rational and irrational numbers are dense on the line, the irrational numbers are much more dense. In fact the rational numbers are infinitely sparse compared to the irrational ones - they form a set of measure zero on any finite interval. What is more, the effect of a perturbation becomes very rapidly smaller as the order of the fraction (ie, the size of M) becomes larger. How this works is seen here for the example of a single pair of frequencies ω_1^0 and ω_2^0, with ratio $T_{12} = \omega_1^0/\omega_2^0$. Then KAM showed that the tori were preserved if

$$\left|\frac{\omega_1^0}{\omega_2^0} - \frac{\alpha}{\beta}\right| > \frac{K(V)}{\beta^{5/2}} \quad (70)$$



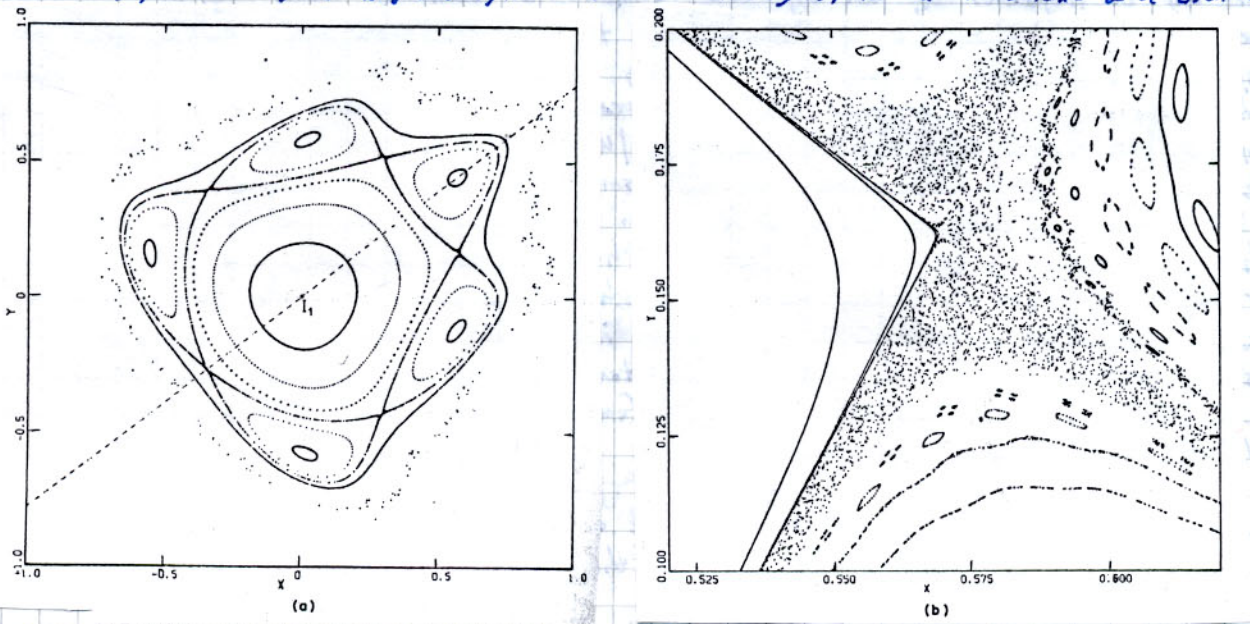
EXCLUDED REGIONS (WHERE CHAOS OCCURS) AROUND A FEW FRACTIONS, ASSUMING $K = 0.5$ (cf. GDTN (70)).

where $K(V)$ is some function that goes to zero with V, and α and β are two integers. The meaning of this is illustrated in the figure on the last page; it is assumed that V and thus $K(V)$ has some small value, and pieces of the real line are cut away around all the rational fractions α/β. (Just a few are shown in the figure). It is easy to see that this leaves most of the real line behind - in fact a crude upper bound to the total length of line that is excised by this procedure is to sum over all α for a given β, and then to sum over all β; this gives for the measure of excised line:

$$\mathcal{M}(K) < \sum_{\beta=1}^{\infty} \beta \frac{K}{\beta^{3/2}} = K \sum_{\beta=1}^{\infty} \frac{1}{\beta^{3/2}} \sim K \qquad (71)$$

This overestimates $\mathcal{M}(K)$ simply because it double-counts a huge number of fractions (eg., the fraction $1/2$ is also counted as $2/4$, $3/6$, $4/8$, etc).

Thus the result of the KAM theorem is that for small perturbations, most invariant tori survive. However there will be regions of phase space where they don't - in these regions, trajectories become "chaotic". This is nicely seen in their "phase portraits", i.e., maps showing where trajectories cross a Poincaré section. The example shown below (with the blow-up at right of the small region around $X = 0.575$, $Y = 0.15$) shows trajectories, for a few different energies, for an anharmonic 2-d oscillator.



(a) Typical phase plane of Henon map with $\alpha = 0.2114$. (b) Blowup of region around right-hand-most hyperbolic point.

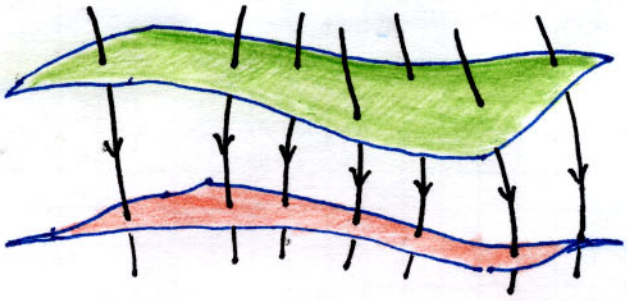
Finally, let's make an elementary deduction from the Hamilton-Jacobi eqtn for a single particle with time-independent Hamiltonian

$$H = \frac{p^2}{2m} + V(\underline{r}) \qquad (72)$$

Then the H-J eqtn (51) becomes, using (53):

$$\boxed{\frac{1}{2m}\left(\nabla S_0(\underline{r})\right)^2 + V(\underline{r}) = E} \qquad (73)$$

i.e., $$|\nabla S_0(\underline{r})| = \sqrt{2m(V-E)} \qquad (74)$$



FLOW OF PARTICLE TRAJECTORIES IN REAL SPACE FOR A PARTICLE, PERPENDICULAR TO SURFACES OF CONSTANT ACTION $S_0(\underline{r})$ = CONSTANT.

It then follows that in real space, the trajectories of particles are perpendicular to the surfaces $S_0(\underline{r}) = \text{const}$. This result was fundamental for both Hamilton (in the application to ray optics) and Schrodinger (in the derivation of wave mechanics).