Chapter 31

Semiclassical evolution

> William Rowan Hamilton was born in 1805. At three he could read English; by four he began to read Latin, Greek and Hebrew, by ten he read Sanskrit, Persian, Arabic, Chaldee, Syrian and sundry Indian dialects. At age seventeen he began to think about optics, and worked out his great principle of "Characteristic Function".
>
> — Turnbull, *Lives of Mathematicians*

(G. Vattay, G. Tanner and P. Cvitanović)

Semiclassical approximations to quantum mechanics are valid in the regime where the de Broglie wavelength $\lambda \sim \hbar/p$ of a particle with momentum p is much shorter than the length scales across which the potential of the system changes significantly. In the short wavelength approximation the particle is a point-like object bouncing off potential walls, the same way it does in the classical mechanics. The novelty of quantum mechanics is the interference of the point-like particle with other versions of itself traveling along different classical trajectories, a feat impossible in classical mechanics. The short wavelength – or semiclassical – formalism is developed by formally taking the limit $\hbar \to 0$ in quantum mechanics in such a way that quantum quantities go to their classical counterparts.

☞ remark 31.1

31.1 Hamilton-Jacobi theory

We saw in chapter 30 that for a 1-dof particle moving in a slowly varying potential, it makes sense to generalize the free particle wave function (30.1) to a wave function

$$\psi(q,t) = A(q,t)e^{iR(q,t)/\hbar}\,, \tag{31.1}$$

with slowly varying (real) amplitude $A(q,t)$ and rapidly varying (real) phase $R(q,t)$. its phase and magnitude. The time evolution of the phase and

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the magnitude of ψ follows from the Schrödinger equation (29.1)

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} - V(q)\right)\psi(q,t) = 0\,. \tag{31.2}$$

Assume $A \neq 0$, and separate out the real and the imaginary parts. We get two equations: The real part governs the time evolution of the phase

$$\frac{\partial R}{\partial t} + \frac{1}{2m}\left(\frac{\partial R}{\partial q}\right)^2 + V(q) - \frac{\hbar^2}{2m}\frac{1}{A}\frac{\partial^2}{\partial q^2}A = 0\,, \tag{31.3}$$

31.8 page 587 and the imaginary part the time evolution of the amplitude

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$$\frac{\partial A}{\partial t} + \frac{1}{m}\sum_{i=1}^{D}\frac{\partial A}{\partial q_i}\frac{\partial R}{\partial q_i} + \frac{1}{2m}A\frac{\partial^2 R}{\partial q^2} = 0\,. \tag{31.4}$$

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In this way a linear PDE for a complex wave function is converted into a set of coupled non-linear PDE's for real-valued functions R and A. The coupling term in (31.3) is, however, of order $\hbar^2$ and thus small in the semiclassical limit $\hbar \to 0$.

Now we generalize the *Wentzel-Kramers-Brillouin* (WKB) *ansatz* for 1-dof dynamics to the Van Vleck *ansatz* in arbitrary dimension: we assume the magnitude $A(q,t)$ varies slowly compared to the phase $R(q,t)/\hbar$, so we drop the $\hbar$-dependent term. In this approximation the phase $R(q,t)$ and the corresponding "momentum field" $\frac{\partial R}{\partial q}(q,t)$ can be determined from the amplitude independent equation

$$\frac{\partial R}{\partial t} + H\left(q, \frac{\partial R}{\partial q}\right) = 0\,. \tag{31.5}$$

In classical mechanics this equation is known as the *Hamilton-Jacobi equation.* We will refer to this step (as well as all leading order in $\hbar$ approximations to follow) as the *semiclassical approximation* to wave mechanics, and from now on work only within this approximation.

31.1.1 Hamilton's equations

We now solve the nonlinear partial differential equation (31.5) in a way the 17 year old Hamilton might have solved it. The main step is the step leading from the nonlinear PDE (31.9) to Hamilton's ODEs (31.10). If you already understand the Hamilton-Jacobi theory, you can safely skip this section.

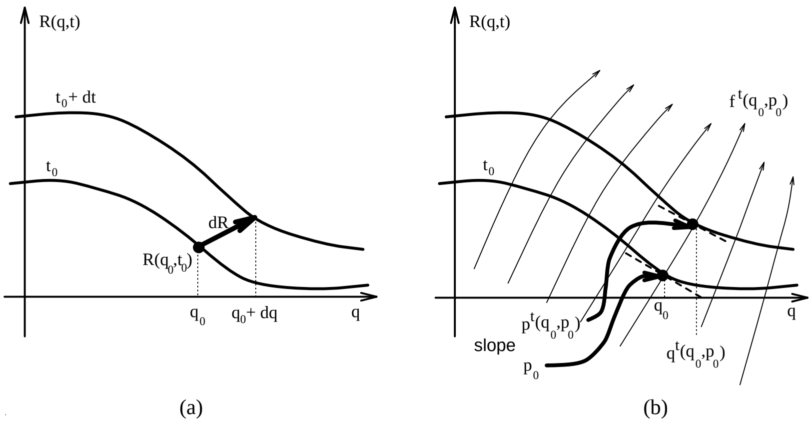

Figure 31.1: (a) A phase $R(q,t)$ plotted as a function of the position q for two infinitesimally close times. (b) The phase $R(q,t)$ transported by a swarm of "particles"; The Hamilton's equations (31.10) construct $R(q,t)$ by transporting $q_0 \to q(t)$ and the slope of $R(q_0,t_0)$, that is $p_0 \to p(t)$.

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The wave equation (29.1) describes how the wave function ψ evolves with time, and if you think of ψ as an (infinite dimensional) vector, position q plays a role of an index. In one spatial dimension the phase R plotted as a function of the position q for two different times looks something like figure 31.1 (a): The phase $R(q,t_0)$ deforms smoothly with time into the phase $R(q,t)$ at time t. Hamilton's idea was to let a swarm of particles transport R and its slope $\partial R/\partial q$ at q at initial time $t = t_0$ to a corresponding $R(q,t)$ and its slope at time t, figure 31.1 (b). For notational convenience, define

$$p_i = p_i(q,t) := \frac{\partial R}{\partial q_i}\,, \quad i = 1, 2, \ldots, D\,. \tag{31.6}$$

We saw earlier that (31.3) reduces in the semiclassical approximation to the Hamilton-Jacobi equation (31.5). To make life simple, we shall assume throughout this chapter that the Hamilton's function $H(q,p)$ does not depend explicitly on time t, i.e., the energy is conserved.

To start with, we also assume that the function $R(q,t)$ is smooth and well defined for every q at the initial time t. This is true for sufficiently short times; as we will see later, R develops folds and becomes multi-valued as t progresses. Consider now the variation of the function $R(q,t)$ with respect to independent infinitesimal variations of the time and space coordinates dt and dq, figure 31.1 (a)

$$dR = \frac{\partial R}{\partial t} dt + \frac{\partial R}{\partial q} dq\,. \tag{31.7}$$

Dividing through by dt and substituting (31.5) we obtain the total derivative of $R(q,t)$ with respect to time *along the as yet arbitrary direction* $\dot{q}$, that is,

$$\frac{dR}{dt}(q,\dot{q},t) = -H(q,p) + \dot{q}\cdot p\,. \tag{31.8}$$

Note that the "momentum" $p = \partial R/\partial q$ is a well defined function of q and t. In order to integrate $R(q,t)$ with the help of (31.8) we also need to know how $p = \partial R/\partial q$ changes along $\dot{q}$. Varying p with respect to independent infinitesimal variations dt and dq and substituting the Hamilton-Jacobi equation (31.5) yields

$$d\frac{\partial R}{\partial q} = \frac{\partial^2 R}{\partial q \partial t}dt + \frac{\partial^2 R}{\partial q^2}dq = -\left(\frac{\partial H}{\partial q} + \frac{\partial H}{\partial p}\frac{\partial p}{\partial q}\right)dt + \frac{\partial p}{\partial q}dq\,.$$

Note that $H(q,p)$ depends on q also through $p(q,t) = \partial R/\partial q$, hence the $\frac{\partial H}{\partial p}$ term in the above equation. Dividing again through by dt we get the time derivative of $\partial R/\partial q$, that is,

$$\dot{p}(q,\dot{q},t) + \frac{\partial H}{\partial q} = \left(\dot{q} - \frac{\partial H}{\partial p}\right)\frac{\partial p}{\partial q}\,. \tag{31.9}$$

Time variation of p depends not only on the yet unknown $\dot{q}$, but also on the second derivatives of R with respect to q with yet unknown time dependence. However, if we *choose* $\dot{q}$ (which was arbitrary, so far) such that the right hand side of the above equation vanishes, we can calculate the function $R(q,t)$ along a specific trajectory $(q(t), p(t))$ given by integrating the ordinary differential equations

$$\dot{q} = \frac{\partial H(q,p)}{\partial p}, \qquad \dot{p} = -\frac{\partial H(q,p)}{\partial q} \tag{31.10}$$

with initial conditions

$$q(t_0) = q', \qquad p(t_0) = p' = \frac{\partial R}{\partial q}(q', t_0). \tag{31.11}$$

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We recognize (31.10) as Hamilton's equations of motion of classical mechanics. The miracle happens in the step leading from (31.5) to (31.9) – if you missed it, you have missed the point. Hamilton derived his equations contemplating optics - it took him three more years to realize that all of Newtonian dynamics can be profitably recast in this form.

$\dot{q}$ is no longer an independent function, and the phase $R(q,t)$ can now be computed by integrating equation (31.8) along the trajectory $(q(t), p(t))$

$$\begin{aligned} R(q,t) &= R(q',t_0) + R(q,t;q',t_0) \\ R(q,t;q',t_0) &= \int_{t_0}^{t} d\tau\,[\dot{q}(\tau)\cdot p(\tau) - H(q(\tau),p(\tau))]\,, \end{aligned} \tag{31.12}$$

with the initial conditions (31.11). In this way the Hamilton-Jacobi *partial* differential equation (31.3) is solved by integrating a set of *ordinary* differential equations, Hamilton's equations. In order to determine $R(q,t)$ for arbitrary q and t we have to find a q' such that the trajectory starting in $(q', p' = \partial_q R(q', t_0))$ reaches q in time t and then compute R along this trajectory, see figure 31.1 (b). The integrand of (31.12) is known as the *Lagrangian*,

$$L(q, \dot{q}, t) = \dot{q} \cdot p - H(q, p, t) . \tag{31.13}$$

A variational principle lurks here, but we shall not make much fuss about it as yet.

Throughout this chapter we assume that the energy is conserved, and that the only time dependence of $H(q,p)$ is through $(q(\tau), p(\tau))$, so the value of $R(q, t; q', t_0)$ does not depend on t_0, but only on the elapsed time $t - t_0$. To simplify notation we will set $t_0 = 0$ and write

$$R(q, q', t) = R(q, t; q', 0) .$$

The initial momentum of the particle must coincide with the initial momentum of the trajectory connecting q' and q:

$$p' = \frac{\partial}{\partial q'} R(q', 0) = -\frac{\partial}{\partial q'} R(q, q', t). \tag{31.14}$$

The function $R(q, q', t)$ is known as *Hamilton's principal function*.

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To summarize: Hamilton's achievement was to trade in the Hamilton-Jacobi *partial* differential equation (31.5) describing the evolution of a wave front for a finite number of *ordinary* differential equations of motion, with the initial phase $R(q, 0)$ incremented by the integral (31.12) evaluated along the phase space trajectory $(q(\tau), p(\tau))$.

31.1.2 Action

Before proceeding, we note in passing a few facts about Hamiltonian dynamics that will be needed for the construction of semiclassical Green's functions. If the energy is conserved, the $\int H(q,p) d\tau$ integral in (31.12) is simply Et. The first term, or the *action*

$$S(q, q', E) = \int_0^t d\tau \, \dot{q}(\tau) \cdot p(\tau) = \int_{q'}^{q} dq \cdot p \tag{31.15}$$

is integrated along a trajectory from q' to q with a fixed energy E. By (31.12) the action is a Legendre transform of Hamilton's principal function

$$S(q, q', E) = R(q, q', t) + Et . \tag{31.16}$$

The time of flight t along the trajectory connecting $q' \to q$ with fixed energy E is given by

$$\frac{\partial}{\partial E} S(q, q', E) = t \,. \tag{31.17}$$

The way to think about the formula (31.16) for action is that the time of flight is a function of the energy, $t = t(q, q', E)$. The left hand side is explicitly a function of E; the right hand side is an implicit function of E through energy dependence of the flight time t.

Going in the opposite direction, the energy of a trajectory $E = E(q, q', t)$ connecting $q' \to q$ with a given time of flight t is given by the derivative of Hamilton's principal function

$$\frac{\partial}{\partial t} R(q, q', t) = -E \,, \tag{31.18}$$

and the second variations of R and S are related in the standard way of Legendre transforms:

$$\frac{\partial^2}{\partial t^2} R(q, q', t) \frac{\partial^2}{\partial E^2} S(q, q', E) = -1 \,. \tag{31.19}$$

A geometric visualization of what the phase evolution looks like is very helpful in understanding the origin of topological indices to be introduced in what follows. Given an initial phase $R(q, t_0)$, the gradient $\partial_q R$ defines a D-dimensional *Lagrangian manifold* $(q,\, p = \partial_q R(q))$ in the full $2d$ dimensional phase space (q, p). The defining property of this manifold is that any contractible loop γ in it has zero action,

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$$0 = \oint_\gamma dq \cdot p,$$

a fact that follows from the definition of p as a gradient, and the Stokes theorem. Hamilton's equations of motion preserve this property and map a Lagrangian manifold into a Lagrangian manifold at a later time. t

Returning back to the main line of our argument: so far we have determined the wave function phase $R(q, t)$. Next we show that the velocity field given by the Hamilton's equations together with the continuity equation determines the amplitude of the wave function.

31.1.3 Density evolution

To obtain the full solution of the Schrödinger equation (29.1), we also have to integrate (31.4).

$$\rho(q, t) := A^2 = \psi^* \psi$$

plays the role of a density. To the leding order in $\hbar$, the gradient of R may be interpreted as the semiclassical momentum density

$$\psi(q,t)^*(-i\hbar\frac{\partial}{\partial q})\psi(q,t) \;=\; -i\hbar A\frac{\partial A}{\partial q}+\rho\frac{\partial R}{\partial q}\,.$$

Evaluated along the trajectory $(q(t),p(t))$, the amplitude equation (31.4) is equivalent to the continuity equation (14.36) after multiplying (31.4) by $2A$, that is

$$\frac{\partial\rho}{\partial t}+\frac{\partial}{\partial q_i}(\rho v_i)=0\,. \tag{31.20}$$

Here, $v_i=\dot{q}_i=p_i/m$ denotes a velocity field, which is in turn determined by the gradient of $R(q,t)$, or the *Lagrangian manifold* $(q(t),p(t)=\partial_q R(q,t))$,

$$v=\frac{1}{m}\frac{\partial}{\partial q}R(q,t).$$

As we already know how to solve the Hamilton-Jacobi equation (31.5), we can also solve for the density evolution as follows:

The density $\rho(q)$ can be visualized as the density of a configuration space flow $q(t)$ of a swarm of hypothetical particles; the trajectories $q(t)$ are solutions of Hamilton's equations with initial conditions given by $(q(0)=q',p(0)=p'=\partial_q R(q',0))$.

If we take a small configuration space volume d^Dq around some point q at time t, then the number of particles in it is $\rho(q,t)d^Ddq$. They started initially in a small volume d^Dq' around the point q' of the configuration space. For the moment, we assume that there is only one solution, the case of several paths will be considered below. The number of particles at time t in the volume is the same as the number of particles in the initial volume at $t=0$,

$$\rho(q(t),t)d^Dq=\rho(q',0)d^Dq'\,,$$

see figure 31.2. The ratio of the initial and the final volumes can be expressed as

$$\rho(q(t),t)=\left|\det\frac{\partial q'}{\partial q}\right|\rho(q',0)\,. \tag{31.21}$$

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As we know how to compute trajectories $(q(t),p(t))$, we know how to compute this Jacobian and, by (31.21), the density $\rho(q(t),t)$ at time t.

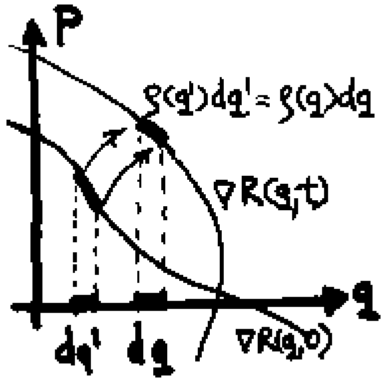

Figure 31.2: Density evolution of an initial surface $(q', p' = \partial_q R(q', 0)$ into $(q(t), p(t))$ surface time t later, sketched in 1 dimension. While the number of trajectories and the phase space Liouville volume are conserved, the density of trajectories projected on the q coordinate varies; trajectories which started in dq' at time zero end up in the interval dq.

31.1.4 Semiclassical wave function

Now we have all ingredients to write down the semiclassical wave function at time t. Consider first the case when our initial wave function can be written in terms of single-valued functions $A(q', 0)$ and $R(q', 0)$. For sufficiently short times, $R(q, t)$ will remain a single-valued function of q, and every $d^D q$ configuration space volume element keeps its orientation. The evolved wave function is in the semiclassical approximation then given by

$$\begin{aligned} \psi_{sc}(q,t) &= A(q,t) e^{iR(q,t)/\hbar} = \sqrt{\det \frac{\partial q'}{\partial q}}\, A(q',0) e^{i(R(q',0)+R(q,q',t))/\hbar} \\ &= \sqrt{\det \frac{\partial q'}{\partial q}}\, e^{iR(q,q',t)/\hbar}\, \psi(q',0)\,. \end{aligned}$$

As the time progresses the Lagrangian manifold $\partial_q R(q, t)$ can develop folds, so for longer times the value of the phase $R(q, t)$ is not necessarily unique; in general more than one trajectory will connect points q and q' with different phases $R(q, q', t)$ accumulated along these paths, see figure 31.3.

We thus expect in general a collection of different trajectories from q' to q which we will index by j, with different phase increments $R_j(q, q', t)$. The hypothetical particles of the density flow at a given configuration space point can move with different momenta $p = \partial_q R_j(q, t)$. This is not an ambiguity, since in the full (q, p) phase space each particle follows its own trajectory with a unique momentum.

Whenever the Lagrangian manifold develops a fold, the density of the phase space trajectories in the fold projected on the configuration coordinates diverges. As illustrated in figure 31.3, when the Lagrangian manifold develops a fold at $q = q_1$; the volume element dq_1 in the neighborhood of the folding point is proportional to $\sqrt{dq'}$ instead of dq'. The Jacobian $\partial q'/\partial q$ diverges like $1/\sqrt{q_1 - q(t)}$ when computed along the trajectory going trough the folding point at q_1. After the folding the orientation of the interval dq' has changed when being mapped into dq_2; in addition the function R, as well as its derivative which defines the Lagrangian manifold, becomes multi-valued. Distinct trajectories starting from different initial

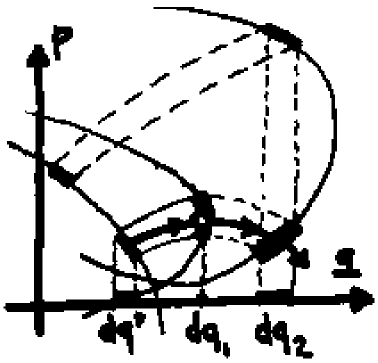

Figure 31.3: Folding of the Lagrangian surface $(q, \partial_q R(q,t))$.

points q' can now reach the same final point q_2. (That is, the point q' may have more than one pre-image.) The projection of a simple fold, or of an envelope of a family of phase space trajectories, is called a *caustic*; this expression comes from the Greek word for "capable of burning", evoking the luminous patterns that one observes swirling across the bottom of a swimming pool.

The folding also changes the orientation of the pieces of the Lagrangian manifold $(q, \partial_q R(q,t))$ with respect to the initial manifold, so the eigenvalues of the Jacobian determinant change sign at each fold crossing. We can keep track of the signs by writing the Jacobian determinant as

$$\det \frac{\partial q'}{\partial q}\bigg|_j = e^{-i\pi m_j(q,q',t)} \left|\det \frac{\partial q'}{\partial q}\right|_j ,$$

where $m_j(q,q',t)$ counts the number of sign changes of the Jacobian determinant on the way from q' to q along the trajectory indexed with j, see figure 31.3. We shall refer to the integer $m_j(q,q',t)$ as the *topological* of the trajectory. So in general the semiclassical approximation to the wave function is thus a sum over possible trajectories that start at any inital q' and end in q in time t

$$\psi_{sc}(q,t) = \int dq' \sum_j \left|\det \frac{\partial q'}{\partial q}\right|_j^{1/2} e^{iR_j(q,q',t)/\hbar - i\pi m_j(q,q',t)/2} \psi(q'_j, 0) \,, \qquad (31.22)$$

each contribution weighted by corresponding density, phase increment and the topological index.

That the correct topological index is obtained by simply counting the number of eigenvalue sign changes and taking the square root is not obvious - the careful argument requires that quantum wave functions evaluated across the folds remain single valued.

31.2 Semiclassical propagator

We saw in chapter 29 that the evolution of an initial wave function $\psi(q,0)$ is completely determined by the propagator (29.12). As $K(q,q',t)$ itself satisfies the Schrödinger equation (29.14), we can treat it as a wave function parameterized by the configuration point q'. In order to obtain a semiclassical approximation to the propagator we follow now the ideas developed in the last section. There is, however, one small complication: the initial condition (29.15) demands that the propagator at $t = 0$ is a δ-function at $q = q'$, that is, the amplitude is infinite at q' and the phase is not well defined. Our hypothetical cloud of particles is thus initially localized at $q = q'$ with *any* initial velocity. This is in contrast to the situation in the previous section where we assumed that the particles at a given point q have well defined velocity (or a discrete set of velocities) given by $\dot{q} = \partial_p H(q, p)$. We will now derive at a semiclassical expression for $K(q, q', t)$ by considering the propagator for short times first, and extrapolating from there to arbitrary times t.

31.2.1 Short time propagator

For infinitesimally short times δt away from the singular point $t = 0$ we assume that it is again possible to write the propagator in terms of a well defined phase and amplitude, that is

$$K(q, q', \delta t) = A(q, q', \delta t) e^{\frac{i}{\hbar} R(q,q',\delta t)} .$$

As all particles start at $q = q'$, $R(q, q', \delta t)$ will be of the form (31.12), that is

$$R(q, q', \delta t) = p\dot{q}\delta t - H(q, p)\delta t , \tag{31.23}$$

with $\dot{q} \approx (q - q')/\delta t$. For Hamiltonians of the form (29.2) we have $\dot{q} = p/m$, which leads to

$$R(q, q', \delta t) = \frac{m(q - q')^2}{2\delta t} - V(q)\delta t .$$

Here V can be evaluated any place along the trajectory from q to q', for example at the midway point $V((q + q')/2)$. Inserting this into our ansatz for the propagator we obtain

$$K_{sc}(q, q', \delta t) \approx A(q, q', \delta t) e^{\frac{i}{\hbar}\left(\frac{m}{2\delta t}(q-q')^2 - V(q)\delta t\right)} . \tag{31.24}$$

For infinitesimal times we can neglect the term $V(q)\delta t$, so $K_{sc}(q, q', \delta t)$ is a d-dimensional Gaussian with width $\sigma^2 = i\hbar\delta t/m$. This Gaussian is a finite width approximation to the Dirac delta function

$$\delta(z) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-z^2/2\sigma^2} \tag{31.25}$$

if $A = (m/2\pi i\hbar\delta t)^{D/2}$, with $A(q, q', \delta t)$ fixed by the Dirac delta function
31.2 normalization condition. The correctly normalized propagator for infinitesimal
586 times δt is therefore

$$K_{sc}(q, q', \delta t) \approx \left(\frac{m}{2\pi i\hbar\delta t}\right)^{D/2} e^{\frac{i}{\hbar}\left(\frac{m(q-q')^2}{2\delta t} - V(q)\delta t\right)} . \tag{31.26}$$

The short time dynamics of the Lagrangian manifold $(q, \partial_q R)$ which corresponds to the quantum propagator can now be deduced from (31.23); one obtains

$$\frac{\partial R}{\partial q} = p \approx \frac{m}{\delta t}(q - q') ,$$

i.e., is the particles start for short times on a Lagrangian manifold which is a plane in phase space, see figure 31.4. Note, that for $\delta t \to 0$, this plane is given by the condition $q = q'$, that is, particles start on a plane parallel to the momentum axis. As we have already noted, all particles start at $q = q'$ but with different velocities for $t = 0$. The inital surface $(q', p' = \partial_q R(q', 0))$ is mapped into the surface $(q(t), p(t))$ some time t later. The slope of the Lagrangian plane for a short finite time is given as

$$\frac{\partial p_i}{\partial q_j} = -\frac{\partial^2 R}{\partial q_j \partial q'_i} = -\frac{\partial p'_i}{\partial q_j} = \frac{m}{\delta t}\delta_{ij} .$$

The prefactor $(m/\delta t)^{D/2}$ in (31.26) can therefore be interpreted as the determinant of the Jacobian of the transformation from final position coordinates q to initial momentum coordinates p', that is

$$K_{sc}(q, q', \delta t) = \frac{1}{(2\pi i\hbar)^{D/2}} \left(\det\frac{\partial p'}{\partial q}\right)^{1/2} e^{iR(q,q',\delta t)/\hbar}, \tag{31.27}$$

where

$$\left.\frac{\partial p'_i}{\partial q_j}\right|_{t,q'} = \frac{\partial^2 R(q, q', \delta t)}{\partial q_j \partial q'_i} \tag{31.28}$$

The subscript $\cdots|_{t,q'}$ indicates that the partial derivatives are to be evaluated with t, q' fixed.

The propagator in (31.27) has been obtained for short times. It is, however, already more or less in its final form. We only have to evolve our short time approximation of the propagator according to (31.22)

$$K_{sc}(q'', q', t' + \delta t) = \sum_j \left|\det\frac{\partial q}{\partial q''}\right|_j^{1/2} e^{iR_j(q'',q,t')/\hbar - i\pi m_j(q'',q,t')/2} K(q, q'_j, \delta t) ,$$

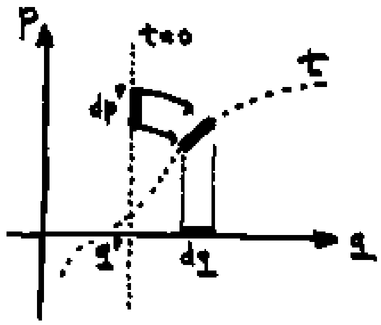

Figure 31.4: Evolution of the semiclassical propagator. The configuration which corresponds to the initial conditions of the propagator is a Lagrangian manifold $q = q'$, that is, a plane parallel to the p axis. The hypothetical particles are thus initially all placed at q' but take on all possible momenta p'. The Jacobian matrix C (31.29) relates an initial volume element in momentum space dp' to a final configuration space volume dq.

and we included here already the possibility that the phase becomes multi-valued, that is, that there is more than one path from q' to q''. The topological index $m_j = m_j(q'', q', t)$ is the number of singularities in the Jacobian along the trajectory j from q' to q''. We can write $K_{sc}(q'', q', t'+\delta t)$ in closed form using the fact that $R(q'', q, t') + R(q, q', \delta t) = R(q'', q', t' + \delta t)$ and the multiplicativity of Jacobian determinants, that is

$$\det \left.\frac{\partial q}{\partial q''}\right|_t \det \left.\frac{\partial p'}{\partial q}\right|_{q',\delta t} = \det \left.\frac{\partial p'}{\partial q''}\right|_{q',t'+\delta t} . \tag{31.29}$$

The final form of the semiclassical or *Van Vleck propagator*, is thus

$$K_{sc}(q, q', t) = \sum_j \frac{1}{(2\pi i\hbar)^{D/2}} \left|\det \frac{\partial p'}{\partial q}\right|^{1/2} e^{iR_j(q,q',t)/\hbar - im_j\pi/2} . \tag{31.30}$$

This Van Vleck propagator is the essential ingredient of the semiclassical quantization to follow.

The apparent simplicity of the semiclassical propagator is deceptive. The wave function is not evolved simply by multiplying by a complex number of magnitude $\sqrt{\det \partial p'/\partial q}$ and phase $R(q, q', t)$; the more difficult task in general is to find the trajectories connecting q' and q in a given time t.

In addition, we have to treat the approximate propagator (31.30) with some care. Unlike the full quantum propagator, which satisfies the group property (29.13) exactly, the semiclassical propagator performs this only approximately, that is

$$K_{sc}(q, q', t_1 + t_2) \approx \int dq''\, K_{sc}(q, q'', t_2) K_{sc}(q'', q', t_1) . \tag{31.31}$$

The connection can be made explicit by the stationary phase approximation, sect. 30.2. Approximating the integral in (31.31) by integrating only over regions near points q'' at which the phase is stationary, leads to the stationary phase condition

$$\frac{\partial R(q, q'', t_2)}{\partial q''_i} + \frac{\partial R(q'', q', t_1)}{\partial q''_i} = 0. \tag{31.32}$$

Classical trajectories contribute whenever the final momentum for a path from q' to q'' and the initial momentum for a path from q'' to q coincide. Unlike the classical evolution of sect. 15.2, the semiclassical evolution is not an evolution by linear operator multiplication, but evolution supplemented by a stationary phase condition $p_{out} = p_{in}$ that matches up the classical momenta at each evolution step.

31.2.2 Free particle propagator

To develop some intuition about the above formalism, consider the case of a free particle. For a free particle the potential energy vanishes, the kinetic energy is $\frac{m}{2}\dot{q}^2$, and the Hamilton's principal function (31.12) is

$$R(q, q', t) = \frac{m(q-q')^2}{2t} \,. \tag{31.33}$$

The weight $\det \frac{\partial p'}{\partial q}$ from (31.28) can be evaluated explicitly, and the Van Vleck propagator is

$$K_{sc}(q, q', t) = \left(\frac{m}{2\pi i\hbar t}\right)^{D/2} e^{im(q-q')^2/2\hbar t} \,, \tag{31.34}$$

identical to the short time propagator (31.26), with $V(q) = 0$. This case is rather exceptional: for a free particle the semiclassical propagator turns out to be the exact quantum propagator $K(q, q', t)$, as can be checked by substitution in the Schrödinger equation (31.2). The Feynman path integral formalism uses this fact to construct an exact quantum propagator by integrating the free particle propagator (with $V(q)$ treated as constant for short times) along all possible (not necessarily classical) paths from q' to q.

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31.3 Semiclassical Green's function

So far we have derived semiclassical formulas for the time evolution of wave functions, that is, we obtained approximate solutions to the time dependent Schrödinger equation (29.1). Even though we assumed in the calculation a time independent Hamiltonian of the special form (29.2), the derivation would lead to the same final result (31.30) were one to consider more complicated or explicitly time dependent Hamiltonians. The propagator is thus important when we are interested in finite time quantum mechanical effects. For time independent Hamiltonians, the time dependence of the propagator as well as of wave functions is, however, essentially given in terms of the energy eigen-spectrum of the system, as in (29.10). It is therefore advantageous to switch from a time representation to an energy representation, that is from the propagator (29.12) to the energy dependent

Green's function (29.16). A semiclassical approximation of the Green's function $G_{sc}(q, q', E)$ is given by the Laplace transform (29.16) of the Van Vleck propagator $K_{sc}(q, q', t)$:

$$G_{sc}(q, q', E) = \frac{1}{i\hbar} \int_0^\infty dt\, e^{iEt/\hbar} K_{sc}(q, q', t)\,. \tag{31.35}$$

The expression as it stands is not very useful; in order to evaluate the integral, at least to the leading order in $\hbar$, we need to turn to the method of stationary phase again.

31.3.1 Stationary phase in higher dimensions

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Generalizing the method of sect. 30.2 to d dimensions, consider stationary phase points fulfilling

$$\left.\frac{d}{dx_i}\Phi(x)\right|_{x=x_0} = 0 \quad \forall i = 1, \dots d\,.$$

An expansion of the phase up to second order involves now the symmetric matrix of second derivatives of $\Phi(x)$, that is

$$D_{ij}(x_0) = \left.\frac{\partial^2}{\partial x_i \partial x_j}\Phi(x)\right|_{x=x_0}\,.$$

After choosing a suitable coordinate system which diagonalizes D, we can approximate the d-dimensional integral by d one-dimensional Fresnel integrals; the stationary phase estimate of (30.13) is then

$$I \approx \sum_{x_0} (2\pi i/s)^{d/2} \left|\det D(x_0)\right|^{-1/2} A(x_0)\, e^{is\Phi(x_0) - \frac{i\pi}{2} m(x_0)}\,, \tag{31.36}$$

where the sum runs over all stationary phase points x_0 of $\Phi(x)$ and $m(x_0)$ counts the number of negative eigenvalues of $D(x_0)$.

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The stationary phase approximation is all that is needed for the semiclassical approximation, with the proviso that D in (31.36) has no zero eigenvalues.

31.3.2 Long trajectories

When evaluating the integral (31.35) approximately we have to distinguish between two types of contributions: those coming from stationary points of the phase and those coming from infinitesimally short times. The first type of contributions can be obtained by the stationary phase approximation and will be treated in this section. The latter originate from the singular behavior of the propagator for $t \to 0$ where the assumption that the amplitude changes slowly compared to the phase is not valid. The short time contributions therefore have to be treated separately, which we will do in sect. 31.3.3.

The stationary phase points t^* of the integrand in (31.35) are given by the condition

$$\frac{\partial}{\partial t} R(q, q', t^*) + E = 0 \,. \tag{31.37}$$

We recognize this condition as the solution of (31.18), the time $t^* = t^*(q, q', E)$ in which a particle of energy E starting out in q' reaches q. Taking into account the second derivative of the phase evaluated at the stationary phase point,

$$R(q, q', t) + Et = R(q, q', t^*) + Et^* + \frac{1}{2}(t - t^*)^2 \frac{\partial^2}{\partial t^2} R(q, q', t^*) + \cdots$$

the stationary phase approximation of the integral corresponding to a classical trajectory j in the Van Vleck propagator sum (31.30) yields

$$G_j(q, q', E) = \frac{1}{i\hbar(2i\pi\hbar)^{(D-1)/2}} \left| \det C_j \left(\frac{\partial^2 R_j}{\partial t^2} \right)^{-1} \right|^{1/2} e^{\frac{i}{\hbar} S_j - \frac{i\pi}{2} m_j} \,, \tag{31.38}$$

where $m_j = m_j(q, q', E)$ now includes a possible additional phase arising from the time stationary phase integration (30.16), and $C_j = C_j(q, q', t^*)$, $R_j = R_j(q, q', t^*)$ are evaluated at the transit time t^*. We re-express the phase in terms of the energy dependent action (31.16)

$$S(q, q', E) = R(q, q', t^*) + Et^* \,, \qquad \text{with} \quad t^* = t^*(q, q', E) \,, \tag{31.39}$$

the Legendre transform of Hamilton's principal function. Note that the partial derivative of the action (31.39) with respect to q_i

$$\frac{\partial S(q, q', E)}{\partial q_i} = \frac{\partial R(q, q', t^*)}{\partial q_i} + \left(\frac{\partial R(q, q', t)}{\partial t^*} + E \right) \frac{\partial t}{\partial q_i} .$$

is equal to

$$\frac{\partial S(q, q', E)}{\partial q_i} = \frac{\partial R(q, q', t^*)}{\partial q_i} , \tag{31.40}$$

due to the stationary phase condition (31.37), so the definition of momentum as a partial derivative with respect to q remains unaltered by the Legendre transform from time to energy domain.

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Next we will simplify the amplitude term in (31.38) and rewrite it as an explicit function of the energy. Consider the $[(D+1)\times(D+1)]$ matrix

$$D(q,q',E) = \begin{pmatrix} \frac{\partial^2 S}{\partial q'\partial q} & \frac{\partial^2 S}{\partial q'\partial E} \\ \frac{\partial^2 S}{\partial q\partial E} & \frac{\partial^2 S}{\partial E^2} \end{pmatrix} = \begin{pmatrix} -\frac{\partial p'}{\partial q} & -\frac{\partial p'}{\partial E} \\ \frac{\partial t}{\partial q} & \frac{\partial t}{\partial E} \end{pmatrix}, \tag{31.41}$$

where $S = S(q,q',E)$ and we used (31.14–31.17) here to obtain the left hand side of (31.41). The minus signs follow from observing from the definition of (31.15) that $S(q,q',E) = -S(q',q,E)$. Note that D is nothing but the Jacobian matrix of the coordinate transformation $(q,E) \to (p',t)$ for fixed q'. We can therefore use the multiplication rules of determinants of Jacobians, which are just ratios of volume elements, to obtain

$$\begin{aligned}\det D &= (-1)^{D+1}\left(\det\frac{\partial(p',t)}{\partial(q,E)}\right)_{q'} = (-1)^{D+1}\left(\det\frac{\partial(p',t)}{\partial(q,t)}\frac{\partial(q,t)}{\partial(q,E)}\right)_{q'} \\ &= (-1)^{D+1}\left(\det\frac{\partial p'}{\partial q}\right)_{t,q'}\left(\det\frac{\partial t}{\partial E}\right)_{q',q} = \det C\left(\frac{\partial^2 R}{\partial t^2}\right)^{-1}.\end{aligned}$$

We use here the notation $(\det .)_{q',t}$ for a Jacobian determinant with partial derivatives evaluated at t, q' fixed, and likewise for other subscripts. Using the relation (31.19) which relates the term $\frac{\partial t}{\partial E}$ to $\partial_t^2 R$ we can write the determinant of D as a product of the Van Vleck determinant (31.28) and the amplitude factor arising from the stationary phase approximation. The amplitude in (31.38) can thus be interpreted as the determinant of a Jacobian of a coordinate transformation which includes time and energy as independent coordinates. This causes the increase in the dimensionality of the matrix D relative to the Van Vleck determinant (31.28).

We can now write down the semiclassical approximation of the contribution of the jth trajectory to the Green's function (31.38) in explicitly energy dependent form:

$$G_j(q,q',E) = \frac{1}{i\hbar(2i\pi\hbar)^{(D-1)/2}}\left|\det D_j\right|^{1/2} e^{\frac{i}{\hbar}S_j - \frac{i\pi}{2}m_j}. \tag{31.42}$$

However, this is still not the most convenient form of the Green's function.

The trajectory contributing to $G_j(q,q',E)$ is constrained to a given energy E, and will therefore be on a phase space manifold of constant energy, that is $H(q,p) = E$. Writing this condition as a partial differential equation for $S(q,q',E)$, that is

$$H(q,\frac{\partial S}{\partial q}) = E,$$

one obtains

$$\begin{aligned}
\frac{\partial}{\partial q_i'} H(q,p) &= 0 = \frac{\partial H}{\partial p_j}\frac{\partial p_j}{\partial q_i'} = \dot{q}_j \frac{\partial^2 S}{\partial q_j \partial q_i'} \\
\frac{\partial}{\partial q_i} H(q',p') &= 0 = \frac{\partial^2 S}{\partial q_i \partial q_j'} \dot{q}_j' \,,
\end{aligned} \tag{31.43}$$

that is the sub-matrix $\partial^2 S/\partial q_i \partial q_j'$ has (left- and right-) eigenvectors corresponding to an eigenvalue 0. Rotate the local coordinate system at the either end of the trajectory

$$(q_1, q_2, q_3, \cdots, q_d) \to (q_\parallel, q_{\perp 1}, q_{\perp 2}, \cdots, q_{\perp (D-1)})$$

so that one axis points along the trajectory and all others are perpendicular to it

$$(\dot{q}_1, \dot{q}_2, \dot{q}_3, \cdots, \dot{q}_d) \to (\dot{q}, 0, 0, \cdots, 0)\,.$$

With such local coordinate systems at both ends, with the longitudinal coordinate axis $q_\parallel$ pointing along the velocity vector of magnitude $\dot{q}$, the stability matrix of $S(q, q', E)$ has a column and a row of zeros as (31.43) takes form

$$\dot{q}\frac{\partial^2 S}{\partial q_\parallel \partial q_i'} = \frac{\partial^2 S}{\partial q_i \partial q_\parallel'}\dot{q}' = 0\,.$$

The initial and final velocities are non-vanishing except for points $|\dot{q}| = 0$. These are the turning points (where all energy is potential), and we assume that neither q nor q' is a turning point (in our application - periodic orbits - we can always chose $q = q'$ not a turning point). In the local coordinate system with one axis along the trajectory and all other perpendicular to it the determinant of (31.41) is of the form

$$\det D(q, q', E) = (-1)^{D+1} \left(\det \begin{matrix} 0 & 0 & \frac{\partial^2 S}{\partial E \partial q_\parallel'} \\ 0 & \frac{\partial^2 S}{\partial q_\perp \partial q_\perp'} & * \\ \frac{\partial^2 S}{\partial q_\parallel \partial E} & * & * \end{matrix} \right). \tag{31.44}$$

The corner entries can be evaluated using (31.17)

$$\frac{\partial^2 S}{\partial q_\parallel \partial E} = \frac{\partial}{\partial q_\parallel} t = \frac{1}{\dot{q}}\,, \qquad \frac{\partial^2 S}{\partial E \partial q_\parallel'} = \frac{1}{\dot{q}'}\,.$$

As the $q_\parallel$ axis points along the velocity direction, velocities $\dot{q}$, $\dot{q}'$ are by construction almost always positive non-vanishing numbers. In this way the determinant of the $[(D+1)\times(D+1)]$ dimensional matrix $D(q,q',E)$ can be reduced to the determinant of a $[(D-1)\times(D-1)]$ dimensional *transverse* matrix $D_\perp(q,q',E)$

$$\begin{aligned}\det D(q,q',E) &= \frac{1}{\dot{q}\dot{q}'}\det D_\perp(q,q',E) \\ D_\perp(q,q',E)_{ik} &= -\frac{\partial^2 S(q,q',E)}{\partial q_{\perp i}\partial q'_{\perp k}}\,.\end{aligned} \tag{31.45}$$

Putting everything together we obtain the jth trajectory contribution to the semiclassical Green's function

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$$G_j(q,q',E) = \frac{1}{i\hbar(2\pi i\hbar)^{(D-1)/2}}\frac{1}{|\dot{q}\dot{q}'|^{1/2}}\left|\det D_\perp^j\right|^{1/2} e^{\frac{i}{\hbar}S_j-\frac{i\pi}{2}m_j}, \tag{31.46}$$

where the topological index $m_j = m_j(q,q',E)$ now counts the number of changes of sign of $\det D_\perp^j$ along the trajectory j which connects q' to q at energy E.

The endpoint velocities $\dot{q}$, $\dot{q}'$ also depend on (q,q',E) and the trajectory j.

31.3.3 Short trajectories

The stationary phase method cannot be used when t^* is small, both because we cannot extend the integration in (30.16) to $-\infty$, and because the amplitude of $K(q,q',t)$ is divergent. In this case we have to evaluate the integral involving the short time form of the exact quantum mechanical propagator (31.26)

$$G_0(q,q',E) = \frac{1}{i\hbar}\int_0^\infty dt\left(\frac{m}{2\pi i\hbar t}\right)^{D/2} e^{\frac{i}{\hbar}\left(\frac{m(q-q')^2}{2t}-V(q)t+Et\right)}\,. \tag{31.47}$$

By introducing a dimensionless variable $\tau = t\sqrt{2m(E-V(q))}/m|q-q'|$, the integral can be rewritten as

$$G_0(q,q',E) = \frac{m}{i\hbar^2(2\pi i)^{D/2}}\left(\frac{\sqrt{2m(E-V)}}{\hbar|q-q'|}\right)^{\frac{D}{2}-1}\int_0^\infty\frac{d\tau}{\tau^{D/2}}e^{\frac{i}{2\hbar}S_0(q,q',E)(\tau+1/\tau)},$$

where $S_0(q,q',E) = \sqrt{2m(E-V)}|q-q'|$ is the short distance form of the action. Using the integral representation of the Hankel function of first kind

$$H_\nu^+(z) = -\frac{i}{\pi}e^{-i\nu\pi/2}\int_0^\infty e^{\frac{1}{2}iz(\tau+1/\tau)}\tau^{-\nu-1}d\tau$$

we can write the short distance form of the Green's function as

$$G_0(q,q',E) \approx -\frac{im}{2\hbar^2}\left(\frac{\sqrt{2m(E-V)}}{2\pi\hbar|q-q'|}\right)^{\frac{D-2}{2}} H^+_{\frac{D-2}{2}}(S_0(q,q',E)/\hbar)\,. \quad (31.48)$$

Hankel functions are stabdard, and their the short wavelength asymptotics is described in standard reference books. The short distance Green's function approximation is valid when $S_0(q,q',E) \leq \hbar$.

Commentary

Remark 31.1 Limit $\hbar \to 0$. The semiclassical limit "$\hbar \to 0$" discussed in sect. 31 is a shorthand notation for the limit in which typical quantities like the actions R or S in semiclassical expressions for the propagator or the Green's function become large compared to $\hbar$. In the world that we live in the quantity $\hbar$ is a fixed physical constant whose value [31.8] is $1.054571596(82)\,10^{-34}$ Js.

Remark 31.2 Madelung's fluid dynamics. Already Schrödinger [31.3] noted that

$$\rho = \rho(q,t) := A^2 = \psi^*\psi$$

plays the role of a density, and that the gradient of R may be interpreted as a local semiclassical momentum, as the momentum density is

$$\psi(q,t)^*(-i\hbar\frac{\partial}{\partial q})\psi(q,t) \;=\; -i\hbar A\frac{\partial A}{\partial q} + \rho\frac{\partial R}{\partial q}\,.$$

A very different interpretation of (31.3–31.4) has been given by Madelung [31.2], and then built upon by Bohm [31.6] and others [31.3, 31.7]. Keeping the $\hbar$ dependent term in (31.3), the ordinary differential equations driving the flow (31.10) have to be altered; if the Hamiltonian can be written as kinetic plus potential term $V(q)$ as in (29.2), the $\hbar^2$ term modifies the p equation of motion as

$$\dot{p}_i = -\frac{\partial}{\partial q_i}\left(V(q) + Q(q,t)\right)\,, \quad (31.49)$$

where, for the example at hand,

$$Q(q,t) = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{\rho}}\frac{\partial^2}{\partial q^2}\sqrt{\rho} \quad (31.50)$$

interpreted by Bohm [31.6] as the "quantum potential". Madelung observed that Hamilton's equation for the momentum (31.49) can be rewritten as

$$\frac{\partial v_i}{\partial t} + \left(v\cdot\frac{\partial}{\partial q}\right)v_i = -\frac{1}{m}\frac{\partial V}{\partial q_i} - \frac{1}{m\rho}\frac{\partial}{\partial q_j}\sigma_{ij}\,, \quad (31.51)$$

where $\sigma_{ij} = \frac{\hbar^2\rho}{4m}\frac{\partial^2 \ln\rho}{\partial q_i \partial q_j}$ is the "pressure" stress tensor, $v_i = p_i/m$, and $\rho = A^2$ as defined [31.3] in sect. 31.1.3. We recall that the Eulerian $\frac{\partial}{\partial t} + \frac{\partial q_i}{\partial t}\frac{\partial}{\partial q_i}$ is the ordinary derivative of Lagrangian mechanics, that is $\frac{d}{dt}$. For comparison, the Euler equation for classical hydrodynamics is

$$\frac{\partial v_i}{\partial t} + \left(v \cdot \frac{\partial}{\partial q}\right) v_i = -\frac{1}{m}\frac{\partial V}{\partial q_i} - \frac{1}{m\rho}\frac{\partial}{\partial q_j}(p\delta_{ij})\,,$$

where $p\delta_{ij}$ is the pressure tensor.

The classical dynamics corresponding to quantum evolution is thus that of an "hypothetical fluid" experiencing $\hbar$ and ρ dependent stresses. The "hydrodynamic" interpretation of quantum mechanics has, however, not been very fruitful in practice.

Remark 31.3 Path integrals. The semiclassical propagator (31.30) can also be derived from Feynman's path integral formalism. Dirac was the first to discover that in the short-time limit the quantum propagator (31.34) is exact. Feynman noted in 1946 that one can construct the exact propagator of the quantum Schrödinger equation by formally summing over all possible (and emphatically not classical) paths from q' to q .

Gutzwiller started from the path integral to rederive Van Vleck's semiclassical expression for the propagator; Van Vleck's original derivation is very much in the spirit of what has presented in this chapter. He did, however, not consider the possibility of the formation of caustics or folds of Lagrangian manifolds and thus did not include the topological phases in his semiclassical expression for the propagator. Some 40 years later Gutzwiller [32.4] added the topological indices when deriving the semiclassical propagator from Feynman's path integral by stationary phase conditions.

Résumé

The aim of the semiclassical or short-wavelength methods is to approximate a solution of the Schrödinger equation with a semiclassical wave function

$$\psi_{sc}(q,t) = \sum_j A_j(q,t) e^{iR_j(q,t)/\hbar}\,,$$

accurate to the leading order in $\hbar$. Here the sum is over all classical trajectories that connect the initial point q' to the final point q in time t. "Semi–" refers to $\hbar$, the quantum unit of phase in the exponent. The quantum mechanics enters only through this atomic scale, in units of which the variation of the phase across the classical potential is assumed to be large. "–classical" refers to the rest - both the amplitudes $A_j(q,t)$ and the phases $R_j(q,t)$ - which are determined by the classical Hamilton-Jacobi equations.

In the semiclassical approximation the quantum time evolution operator is given by the *semiclassical propagator*

$$K_{sc}(q,q',t) = \frac{1}{(2\pi i\hbar)^{D/2}} \sum_j \left| \det \frac{\partial p'}{\partial q} \right|_j^{1/2} e^{\frac{i}{\hbar}R_j - \frac{i\pi}{2}m_j} \,,$$

where the topological index $m_j(q,q',t)$ counts the number of the direction reversal along the jth classical trajectory that connects $q' \to q$ in time t. Until very recently it was not possible to resolve quantum evolution on quantum time scales (such as one revolution of electron around a nucleus) - physical measurements are almost always done at time scales asymptotically large compared to the intrinsic quantum time scale. Formally this information is extracted by means of a Laplace transform of the propagator which yields the energy dependent *semiclassical Green's function*

$$\begin{aligned} G_{sc}(q,q',E) &= G_0(q,q',E) + \sum_j G_j(q,q',E) \\ G_j(q,q',E) &= \frac{1}{i\hbar(2\pi i\hbar)^{\frac{(D-1)}{2}}} \left| \frac{1}{\dot{q}\dot{q}'} \det \frac{\partial p'_\perp}{\partial q_\perp} \right|_j^{1/2} e^{\frac{i}{\hbar}S_j - \frac{i\pi}{2}m_j} \end{aligned} \qquad (31.52)$$

where $G_0(q,q',E)$ is the contribution of short trajectories with $S_0(q,q',E) \leq \hbar$, while the sum is over the contributions of long trajectories (31.46) going from q' to q with fixed energy E, with $S_j(q,q',E) \gg \hbar$.

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