Chapter 5

Semiclassical approximation of path integrals

5.1 Gaussian approximation

Semiclassical approximation of a path integral is its (approximate) reduction to a Gaussian form. Since we are going to built the amplitude around a classical trajectory through constructing the quantum mechanical corrections similarly as it was the case for the Gaussian integrals we start by expanding the action around a classical trajectory, $\bar{x}(t)$:

$$
\begin{aligned}
S[x(t)] &= S[\bar{x}(t) + y(t)] = S[\bar{x}] + \delta S[\bar{x}, y] + \frac{1}{2!}\delta^2 S[\bar{x}, y] + \ldots \\
&= S[\bar{x}] + \frac{1}{2!}\int_0^T \left[\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}^2 + 2\frac{\partial^2 L}{\partial x \partial \dot{x}}\dot{y}y + \frac{\partial^2 L}{\partial x^2}y^2\right] dt + \ldots \qquad (5.1)
\end{aligned}
$$

where, similarly as in the case of Gaussian integrals, $y(t)$ is the correction to the classical trajectory. The difference is that now $y(t)$ is assumed to be a small correction (and that is the reason why the higher than quadratic terms in the expansion of S are neglected), whereas there was no such restriction for Gaussian integrals. Clearly, $\delta S = 0$ which leads to the Lagrange equations for $\bar{x}$

$$
\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right) - \frac{\partial L}{\partial x} = 0\,. \qquad (5.2)
$$

When $\hbar \to 0$ the significant contributions to the path integrals come from the trajectories which differ little from the classical trajectory: summation over them is approximately coherent, hence non-destructive because $\delta S[\bar{x}] = 0$.

The validity criterium of our approximation is then: $S[\bar{x}]/\hbar \gg 1$, i.e. $S[\bar{x}]$ dominates in the exponent of the path integral, and $\delta^2 S[\bar{x}, y]/2!$ is the correction:

$$\int [\mathcal{D}x(t)]\, e^{\frac{i}{\hbar}S[x(t)]} \approx e^{\frac{i}{\hbar}S[\bar{x}]} \int\limits_{y(0)=y(t)=0} [\mathcal{D}y(t)]\, e^{\frac{i}{\hbar}\frac{1}{2!}\int\limits_0^T \left[\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}^2 + 2\frac{\partial^2 L}{\partial x \partial \dot{x}}\dot{y}y + \frac{\partial^2 L}{\partial x^2}y^2\right] dt}$$
$$= e^{\frac{i}{\hbar}S[\bar{x}]}\, F(T)\,. \tag{5.3}$$

That is the reason we call this procedure the"semiclassical approximation".

In order to analyze the contribution of the correction factor in (5.3) we present $\delta^2 S$ in a different from given above form. We use the identities:

$$\dot{y}\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y} = \frac{d}{dt}\left(y\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}\right) - y\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}\right)$$
$$2y\frac{\partial^2 L}{\partial x \partial \dot{x}}\dot{y} = \frac{d}{dt}\left(\frac{\partial^2 L}{\partial x \partial \dot{x}}y^2\right) - y\frac{d}{dt}\left(\frac{\partial^2 L}{\partial x \partial \dot{x}}\right)y \tag{5.4}$$

where we must remember that all derivatives of L with respect to x and $\dot{x}$ are taken at the classical trajectory $\bar{x}$. Therefore all the coefficients of y and $\dot{y}$ in (5.4) *are some well defined functions of t one can calculate knowing L and $\bar{x}$*. Remembering that $y(0) = y(T) = 0$ we can, with the help of (5.4), do integrations by parts and obtain:

$$\delta^2 S = \int\limits_0^T \left[\dot{y}\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y} + 2y\frac{\partial^2 L}{\partial x \partial \dot{x}}\dot{y} + y\frac{\partial^2 L}{\partial x^2}y\right] dt$$
$$= -\int\limits_0^T y\left[\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}\right) + \frac{d}{dt}\left(\frac{\partial^2 L}{\partial x \partial \dot{x}}\right)y - \frac{\partial^2 L}{\partial x^2}y\right] dt$$
$$= \int\limits_0^T y\, D(t) y\, dt\,. \tag{5.5}$$

$D(t)$ is the Sturm-Liouville differential operator which, in general, has an infinity of eigenvalues and eigenvectors:

$$D(t)y_n(t) = \lambda_n y_n(t)\,, \quad n = 1, 2, 3, \ldots\,, \quad \lambda_1 < \lambda_2 < \ldots\,. \tag{5.6}$$

Example: Sturm-Liouville Operator for the harmonic oscillator

Let us take $L = \frac{1}{2}m\dot{x}^2 - V(x)$, then

$$D(t) = -m\frac{\partial^2}{\partial t^2} - \left.\frac{\partial^2 V}{\partial x^2}\right|_{x=\bar{x}(t)}\,.$$

This is the same differential operator we had in the equation for $\delta x(t)$ when we calculated the van Vleck prefactor in the preceding section. In the case of the harmonic oscillator we get

$$D(t) = -m\frac{\partial^2}{\partial t^2} - m\omega^2\,,$$

whose eigenvalues are $\lambda_n = m((n\pi/T)^2 - \omega^2)$.

End of Example

Any $y(t)$ vanishing at $t = 0$ and $t = T$ can be expanded in an orthonormal set of $y_n(t)$' s and we get

$$\delta^2 S[y] = \sum_{n=1}^{\infty} \lambda_n a_n^2 \tag{5.7}$$

where a_n's are the expansion coefficients:

$$y(t) = \sum_{n=1}^{\infty} a_n \, y_n(t) \, . \tag{5.8}$$

So, the summation over the trajectories on the r.h.s. of (5.3) is now, because of (5.7), reduced to integrations over a_n's. Thus

$$[\mathcal{D}y(t)] \sim \prod_{n=1}^{\infty} da_n \, , \tag{5.9}$$

and, provided we can solve the eigenvalue problem given by (5.6), we reduce evaluation of the r.h.s. of (5.3) to simple Gaussian integrals, and we have

$$F(T) \sim \sqrt{\frac{1}{\prod_n \lambda_n}} = \sqrt{\frac{1}{\det D(t)}} \, . \tag{5.10}$$

Note the similarities with the exact solutions for the Gaussian path integrals.

The eigenvalues (5.6) and closely related with them the so called Jacobi equation

$$\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}^2}\dot{y}\right) + \frac{d}{dt}\left(\frac{\partial^2 L}{\partial x \partial \dot{x}}\right) y - \frac{\partial^2 L}{\partial x^2} y = 0 \, , \tag{5.11}$$

play an important role in semiclassical approximations to path integrals and it is time now to discuss their properties and applications.

This discussion which follows is in fact just another version of considerations presented above for the Gaussian integrals adapted here for the cases when the Lagrangian is arbitrary (i.e. not necessarily a quadratic form). We follow the formulation of Ref.[5.1] which is a generalisation of the arguments presented above in section **??**.

Similarly as before we consider a family of classical trajectories which start from the space-time point $(a, 0)$ with various momenta p (or velocities v), $x(p, t)$:

$$x(p, 0) = a \, , \qquad \text{for all } \; p \, . \tag{5.12}$$

In order to find a measure of the density of our family of trajectories we introduce

$$\mathcal{N}(p, t) = \frac{\partial x(p, t)}{\partial p} \, . \tag{5.13}$$

Thus the difference between two trajectories whose momenta differ slightly is, to lowest order,

$$x(p+\delta p,t)-x(p,t)=\mathcal{N}(p,t)\delta p\,. \tag{5.14}$$

Thus, indeed, $\mathcal{N}(p,t)$ measures the density of trajectories.

Since each $x(p,t)$ is a solution of the Lagrange equation (5.2), we get the equation for $\mathcal{N}$ by differentiating (5.2) with respect to p, and get again the Jacobi equation:

$$\frac{d}{dt}\left(\frac{\partial^2 L}{\partial \dot{x}^2}\dot{\mathcal{N}}\right)+\frac{d}{dt}\left(\frac{\partial^2 L}{\partial x\partial \dot{x}}\right)\mathcal{N}-\frac{\partial^2 L}{\partial x^2}\mathcal{N}=0\,. \tag{5.15}$$

For a given $x(p,t)$ all derivatives of L taken along this trajectory are well defined functions of time. Because of (5.12), and $p=m\dot{x}(p,0)$, we have the following initial conditions for $\mathcal{N}$:

$$\mathcal{N}(p,0)=0 \qquad \text{and} \qquad \frac{\partial \mathcal{N}(p,0)}{\partial t}=\frac{1}{m}\,. \tag{5.16}$$

A space-time point (b,T) we call *conjugate* to the initial $(a,0)$ when

$$\mathcal{N}(p,T)=\frac{\partial x(p,T)}{\partial p}=0\,. \tag{5.17}$$

Note that there $x(p,T)=b$ does not depend on p (compare (5.17)). Therefore, *all trajectories which started at* $(a,0)$ *coincide at* (b,T). That is why we can call this point a *focal point* (or a "caustic" point, $\kappa\alpha\upsilon\sigma\theta\iota\kappa o\sigma$ = burning). Note also that this condition (5.17) realizes the demand that variation of the initial p does not change $x(T)=b$. Indeed

$$\delta x(p,T)=x(p+\delta p,T)-x(p,T) \;=\; \frac{\partial x(p,T)}{\partial p}\delta p \tag{5.18}$$

which implies (5.14).

Now, we can compare $\mathcal{N}(p,t)$ with $\mathcal{N}$ of section **??**, eq.(**??**). Let (b,T) be an arbitrary space-time endpoint. From the definition (5.13) and identification $x(p,T)=b$ we get

$$\frac{1}{\mathcal{N}(p,T)}=\frac{\partial p}{\partial b}\,. \tag{5.19}$$

On the other hand we can compute p from the action, $S(a,b,T)$, taken along the trajectory $x(p,t)$:

$$p=-\frac{\partial S(a,b,T)}{\partial a}\,. \tag{5.20}$$

Inserting this into (5.19) we finally obtain

$$[\mathcal{N}(p,T)]^{-1}=-\frac{\partial^2 S(a,b,T)}{\partial a\partial b} \tag{5.21}$$

and

$$F=\left(-\frac{1}{2\pi\hbar i}\frac{\partial^2 S(a,b,T)}{\partial a\partial b}\right)^{\frac{1}{2}}\,. \tag{5.22}$$

Thus the two $\mathcal{N}$'s, eqs.(**??**) and (5.13), are the same objects. Note that $-\partial^2 S/\partial a \partial b$ becomes singular at the conjugate (focal) points.

Example: Caustic point of the harmonic oscillator

Application to the harmonic oscillator:

$$\mathcal{N}_{\text{osc}}^{-1} = \frac{m\omega}{\sin \omega T}, \qquad \text{for } \; T = \frac{n\pi}{\omega}, \; n = 0, 1, 2, ... \qquad \mathcal{N}_{\text{osc}} = 0 \,.$$

Thus, since

$$\frac{\partial x_{\text{osc}}(p, n\pi/\omega)}{\partial p} = 0 \qquad \text{for all } \; p \,,$$

all trajectories coincide at these "caustic" points.

End of Example

Now, we relate the above to the properties of the eigenvalues of (5.6). First, let us observe that they depend on T, and, in general, they decrease with increasing T (compare the examples given below). In terms of λ_n's, one can give the following definition of the point $b = \bar{x}(T)$ conjugate to $a = \bar{x}(0)$. These two space-time points define a Sturm–Liouville equation (5.6) and a set of eigenfunctions and eigenvalues. When the smallest eigenvalue becomes zero,

$$\lambda_1(T) = 0 \,, \tag{5.23}$$

b is conjugate to a.

The relation between these two alternative definitions of conjugate points follows from realization that $\mathcal{N}$ and $\prod_{n=1}^{\infty} \lambda_n$ must have the same zeros. Indeed, they appear as factors $(\mathcal{N})^{-\frac{1}{2}}$, or $(\prod_{n=1}^{\infty} \lambda_n)^{-\frac{1}{2}}$, depending on which method is followed in computing the prefactor of the exponent $\exp(iS[\bar{x}]/\hbar)$ in the semiclassical approximation (5.3). So, they lead to the same singularities of the amplitude when b becomes conjugate to a.

One can illustrate these points on the results obtained in section **??** for the harmonic oscillator:

$$\sqrt{\frac{1}{\mathcal{N}}} = \sqrt{\frac{m\omega}{\sin \omega T}} \tag{5.24}$$

and

$$\sqrt{\frac{1}{\prod_n \lambda_n}} = \sqrt{\left[\prod_n m \Big((\frac{n\pi}{T})^2 - \omega^2 \Big) \right]^{-1}} \,. \tag{5.25}$$

Clearly, (5.24) and (5.25) have the same singularities at

$$T = \frac{n\pi}{\omega} \qquad n = 1, 2, 3, \ldots \,. \tag{5.26}$$

Which means that there are infinitely many conjugate (focal) points. The condition (5.23) gives the first of them.

Let us illustrate conjugation and focusing again on the harmonic oscillator case. Let us take (e.g. from section **??**) the trajectory which goes from a to b in time T

$$\bar{x}(t) = \frac{1}{\sin\omega T}\left[b\sin\omega t + a\sin\omega(T-t)\right] . \tag{5.27}$$

So, when $\omega T = n\pi$, we have singularities not only in the propagator but also in the classical trajectory. However, when $b = (-1)^n a$ *the singularities disappear* (show it!). One can check that $K(b, a, T)$ is consistent with above. Indeed, (prove that!)

$$K(b, a, \frac{n\pi}{\omega}) \;=\; e^{-in\frac{\pi}{2}}\,\delta\left(b-(-1)^n a\right) . \tag{5.28}$$

One can also show (show it!) that the harmonic oscillator propagator for arbitrary T is given by the Feynman–Souriau formula ($\left[\frac{T\omega}{\pi}\right] = n$)

$$K(b, a, T) = e^{-i\frac{\pi}{4}}\, e^{-i\frac{\pi}{2}\left[\frac{T\omega}{\pi}\right]}\sqrt{\frac{m\omega}{2\pi\hbar|\sin\omega T|}}\; e^{\frac{im\omega}{2\hbar\sin\omega T}\left[(b^2+a^2)\cos\omega T - 2ab\right]} . \tag{5.29}$$

So, when T hits the "conjugate time-lapse" *it must be* $b = \pm a$.

With the help of (5.27) we can also inspect a family of trajectories (denoted $x(p, t)$ above) starting from $x = a$ with various initial momenta:

$$x(p, t) = \frac{a}{\sin\omega T}\left[(-1)^n\sin\omega t + \sin(\omega T - \omega t)\right] . \tag{5.30}$$

Note that in (5.29) we have, in fact, two families of trajectories: for n even, and for n odd. They differ by the sign of the $\sin\omega t$ term. Their initial conditions are

$$x^{\text{even}}_{\text{odd}}(p, 0) = a\,, \qquad \dot{x}^{\text{even}}_{\text{odd}}(p, 0) = \frac{a\omega}{\sin\omega T}\left[\pm 1 - \cos\omega T\right] . \tag{5.31}$$

Changing T we regulate the initial velocity (momentum). We have now

$$x_{\text{even}}\left(p, \frac{n\pi}{\omega}\right) = x_{\text{odd}}\left(p, \frac{n\pi}{\omega}\right) = (-1)^n a\,. \tag{5.32}$$

Thus all trajectories, irrespective of p and n, go through the same focal points.

So far we have been writing the formulae for the case of one space and one time dimension. They can be generalized to an arbitrary number of spatial dimensions.

Let x be n - dimensional: $x_1, ..., x_i, ..., x_n$. We have also n initial momenta: $p_1, ..., p_k, ..., p_n$. Now, the initial conditions are

$$x_i(p_1, ..., p_k, ..., p_n, t = 0) = a_i, \qquad \text{for all} \;\; p_k\,, \tag{5.33}$$

and our old $\mathcal{N}$ becomes a matrix

$$\mathcal{N}_{ik}(p, t) \;=\; \frac{\partial x_i(p, t)}{\partial p_k}\,, \tag{5.34}$$

where p stands for $p_1, ..., p_k, ..., p_n$. One can show (show it!) that its differential equation is an analogue of (5.15) (we sum over repeated indices):

$$\frac{d}{dt}\left(\frac{\partial^2 L}{\partial\dot{x}_i\partial\dot{x}_l}\dot{\mathcal{N}}_{lk}\right) \;+\; \left(\frac{\partial^2 L}{\partial\dot{x}_i\partial x_l} - \frac{\partial^2 L}{\partial x_i\partial\dot{x}_l}\right)\dot{\mathcal{N}}_{lk}$$

$$+\;\left[\frac{d}{dt}\left(\frac{\partial^2 L}{\partial\dot{x}_i\partial x_l}\right) - \frac{\partial^2 L}{\partial x_i\partial x_l}\right]\mathcal{N}_{lk} \;=\; 0 \tag{5.35}$$

with the same initial conditions as given above for $\mathcal{N}$

$$\mathcal{N}_{ik}(p,0) = 0\,, \qquad \frac{\partial \mathcal{N}_{ik}(p,0)}{\partial t} = \frac{1}{m}\,\delta_{ik}\,. \tag{5.36}$$

The focal point we get demanding that a variation of x_i with respect to all initial p_k's, an analogue of (5.18), be zero when

$$x_i(T) = b_i\,. \tag{5.37}$$

Indeed, making

$$\delta x_i = \sum_k [x_i(...p_k + \delta p_k..., T) - x_i(...p_k..., T)] = \sum_k \frac{\partial x_i}{\partial p_k}\delta p_k = 0\,, \tag{5.38}$$

where all δp_k's are arbitrary but small, we get the following condition for a solution to (5.38) to exist

$$det\left(\frac{\partial x_i}{\partial p_k}\right) \;=\; det\left(\mathcal{N}_{ik}(p,T)\right) \;=\; 0\,. \tag{5.39}$$

This is an analogue to (5.17).

Similarly as it was shown above for one dimensional case we can relate $(\mathcal{N}_{ik})^{-1}$ to the derivatives of the action S. Indeed, from

$$\mathcal{N}_{ik}(p,T) = \frac{\partial x_i(p,T)}{\partial p_k} = \frac{\partial b_i}{\partial p_k}\,, \tag{5.40}$$

we have

$$(\mathcal{N}_{ik})^{-1} = \frac{\partial p_k}{\partial b_i}\,. \tag{5.41}$$

On the other hand we have the relation

$$p_k = -\frac{\partial S(...a_k..., ...b_i..., T)}{\partial a_k} \tag{5.42}$$

and from (5.41) and (5.42) we get

$$(\mathcal{N}_{ik})^{-1} = -\frac{\partial^2 S(...a_k..., ...b_i..., T)}{\partial a_k \partial b_i}\,. \tag{5.43}$$

When the matrix (5.43) is symmetric it has real eigenvalues (this is the case when we have reversibility of classical trajectories, which in the presence of a magnetic field breaks down). These eigenvalues depend on T, in general. These are the eigenvalues we have already discussed which determine the prefactors of the semiclassical approximation of the propagators. The conjugate or focal points occur when one of the eigenvales vanishes. The rate of growth with time T of the largest eigenvalue is called the Liapunoff exponent of the trajectory. When some of the eigenvalues grow exponentially with time we have instabilities. Such a behavior is very different from the stable behavior of e.g. the harmonic oscillator. There, the eigenvalues are bounded for all T. This means that the spatial spread of trajectories is finite at all times. Here, in contrast, the exponentially growing eigenvalues imply infinite spread of the fan of trajectories. In classical physics this means big trouble. Not in quantum physics: when $\lambda_k \to \infty$, $F \to 0$ (see the formula below) and a classically chaotic behavior does not lead to any difficulty. This unstable regime has a vanishing probability amplitude.

Before writing down the complete expression for the propagator in semiclassical approximation we shall discuss how its phase factors come about. The prefactors of such propagators are

$$F \sim \left(\prod_{n=1}^{\infty} \lambda_n\right)^{-\frac{1}{2}} .$$

Therefore, when we want to have $K_{sc}(b, a, T)$ for all T, we have to know the number of eigenvalues λ_n which become negative (this happens at the points conjugate to the initial point). When a λ_n goes through zero it changes sign. Thus the Gaussian integrals which give the prefactor behave as

$$\int da_n\, e^{i|\lambda_n|a_n^2} \;\to\; \int da_n\, e^{-i|\lambda_n|a_n^2} .$$

Therefore each negative eigenvalue contributes the phase $-i = e^{-i\frac{1}{2}\pi}$. In fact all this has a proper mathematical formulation which is based on the so called

Morse theorem:
The second variation, $\delta^2 S = \sum_n \lambda_n a_n^2$, has as many negative eigenvalues as there are conjugate points along the trajectory going from $(a, 0)$ to (b, T).

Note that this theorem implies that, at a conjugate point a λ *changes its sign*, thus *it cannot become zero without changing its sign*. We must remember also that there may be more than one classical trajectory going from $(a, 0)$ to (b, T): e.g. in some topologically nontrivial cases.

Putting all this together we can write the e.g. three dimensional semiclassical propagator $K_{sc}(\mathbf{b}, \mathbf{a}, T)$ as follows:

$$K_{sc}(\mathbf{b}, \mathbf{a}, T) = \sum_{\tau} \left(\frac{i}{2\pi\hbar}\right)^{\frac{3}{2}} e^{-in_\tau \frac{1}{2}\pi} \sqrt{\left|\det \frac{\partial^2 S_\tau}{\partial \mathbf{a} \partial \mathbf{b}}\right|}\, e^{\frac{i}{\hbar} S_\tau(\mathbf{a}, \mathbf{b}, T)} \tag{5.44}$$

where τ labels all possible classical trajectories between $(\mathbf{a}, 0)$ and $(\mathbf{b}, T)$, and n_τ is the number of negative eigenvalues of $\delta^2 S$ along the classical trajectory τ. We can check that the Feynman–Souriau formula (5.29) is a special case of (5.44).

Note that the operation of taking the sum over *classical* trajectories is nevertheless a *quantal* operation: we follow *the superposition principle* which says that any two or more states may be superposed to give a new state.

Note also that the absolute value of det(...) appears because all changes of its sign under the square root are taken care of by the phase factor $\exp(-in_\tau \pi/2)$.

5.2 Consequences of single valuedness of $K(b, a)$

Now, let us discuss the consequences of the single valuedness of the propagator

$$K(b, a, T) \; = \; F(T)\, e^{\frac{i}{\hbar} S(b,a,T)} \, . \tag{5.45}$$

As we know $K(b, a, T)$ is also a wave function $\psi(b, T)$. Therefore we must be dealing with a single valued function $K(b, a, T)$. In other words, starting from b and going along a trajectory *which comes back to* b (once or many times) we must be returning to the same value of K (hence ψ). Intuitively, a classical trajectory which comes back to the same place looks like the one of a bound state.

So, what we are going to seek now is an *energy* which *for a given closed classical trajectory* meets the condition of the uniqueness of $K(b, a, T)$. From the classical mechanics

$$\delta S(b, a, T) \; = \; p_b \delta b - p_a \delta a - E \delta T \, , \tag{5.46}$$

thus

$$p_b = \frac{\partial S(b, a, T)}{\partial b} \, , \qquad p_a = -\frac{\partial S(b, a, T)}{\partial a} \, , \qquad E = -\frac{\partial S(b, a, T)}{\partial T} \, . \tag{5.47}$$

The last of these equations tells us that, for a given trajectory going from a to b in time T, there is a well defined energy $E = E(T)$ (which equation can also be inverted $T = T(E)$).

Thus for a given trajectory with fixed T, E is also fixed. Let us write the action in a somewhat different form, appropriate for trajectories with a given (fixed) energy E.

$$S(b, a, T) = \int_a^b \sum_r p_r dq_r - ET \, . \tag{5.48}$$

One can justify this as follows:

$$\begin{aligned} \int_a^b \sum_r p_r dq_r - ET \; &= \; \int_0^T \sum_r p_r \dot{q}_r dt - \int_0^T H dt \\ &= \int_0^T dt (\sum_r p_r \dot{q}_r - H) = \int_0^T dt L(q_r, \dot{q}_r) = S(b, a, T) \, , \end{aligned}$$

because, by definition

$$H(p_r, q_r) = \sum_r \dot{q}_r \frac{\partial L}{\partial \dot{q}_r} - L \qquad \text{and} \qquad p_r = \frac{\partial L}{\partial \dot{q}_r} \, . \tag{5.49}$$

So, following a closed trajectory of a fixed energy, we change $S \to S + \Delta S$ where

$$\Delta S = \oint \sum_r p_r \, dq_r \, . \tag{5.50}$$

But, as we already know, the prefactor F also changes and, in fact, as we have seen, passing each conjugate point gives us a phase $e^{-i\pi/2}$. Writing

$$K = F\, e^{\frac{i}{\hbar}S} = e^{\ln F + \frac{i}{\hbar}S}\,, \tag{5.51}$$

we see that the change of the exponent amounts to

$$\Delta = \Delta \ln F + \frac{i}{\hbar}\Delta S = -\Delta(i\frac{\pi}{2}) + \frac{i}{\hbar}\oint \sum_r p_r\, dq_r = -mi\frac{\pi}{2} + \frac{i}{\hbar}\oint \sum_r p_r\, dq_r\,,$$

with m being the number of conjugate points along our trajectory. Thus, in order to keep K single valued, we have to have

$$\Delta = 2\pi i n = -mi\frac{\pi}{2} + \frac{i}{\hbar}\oint \sum_r p_r\, dq_r\,, \qquad n = 0, 1, 2, ... \tag{5.52}$$

hence

$$\oint \sum_r p_r\, dq_r = 2\pi\hbar\left(n + \frac{m}{4}\right)\,. \tag{5.53}$$

Note that K would be single valued for $n = 0, \pm 1, \pm 2, \pm 3...$, but one must remember that single valuedness is a *necessary* but not a *sufficient* condition for having physically meanningful solutions. In this specific case the negative n's should be rejected (discuss this point). So, in order to implement the condition of single valuedness, we have to know the number m of conjugate points passed with each circling of one orbit.

5.2.1 Application to harmonic oscillator

Let us apply (5.53) to the harmonic oscillator. We have now

$$E = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2 = \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2 x^2\,. \tag{5.54}$$

Thus the momentum as the function of position, $p(x)$, and the turning points, $\pm x_R$ are

$$p(x) = \pm\sqrt{2mE - m^2\omega^2 x^2}\,, \qquad x_R = \sqrt{\frac{2E}{m\omega^2}}\,. \tag{5.55}$$

Circling one orbit means that we have to go from e.g. $-x_R$ to $+x_R$, and then back to $-x_R$. Remembering that $p(x)$ changes sign in the process we have

$$\oint \sum_r p_r dq_r = 2\int_{-x_R}^{x_R} p(x)dx = 4\frac{E}{\omega}\int_{-1}^{+1} du\sqrt{1-u^2} = 2\pi\frac{E}{\omega}\,. \tag{5.56}$$

Since going from $-x_R$ to $+x_R$ and back takes $T = 2\pi/\omega$ we know from our discussion of the oscillator trajectories given above, that this round trip goes through two conjugate points. Thus m in (5.53) equals 2. Therefore, for the oscillator we obtain

$$\oint pdq = 2\pi\hbar(n + \tfrac{1}{2}) = 2\pi\frac{E}{\omega}\,. \tag{5.57}$$

and the well known formula

$$E = \hbar\omega\left(n + \tfrac{1}{2}\right) . \tag{5.58}$$

Note that the 1/2 in the above formula comes from $m = 2$ for the oscillator. This result for E is exact because L is a Gaussian.

5.2.2 Application to Coulomb potential

Let us discuss some non-Gaussian cases e.g. the Bohr formula for the hydrogen spectrum: an electron moving in Coulomb potential, $-e^2/r$, centered at the infinitely heavy proton (we neglect spin and relativistic corrections). The first thing we must decide about is the number of conjugate points of a closed trajectory. This is known from classical trajectories of the Kepler problem. It was found in [5.5] that there are *four* conjugate points on the Kepler ellipse in three dimensions. Thus in (5.53) we set $m = 4$, and the quantization condition for the Bohr atom becomes

$$\oint \sum_r p_r\, dq_r = 2\pi\hbar\,(n+1)\,, \qquad n = 0, 1, 2, \dots . \tag{5.59}$$

To calculate the l.h.s. of eq.(5.59) let us consider an approximate model of the hydrogen atom. The motion is in the (x, y)-plane. We introduce the polar coordinates

$$x = r\cos\phi\,, \qquad y = r\sin\phi\,. \tag{5.60}$$

The Lagrangian is

$$L = \tfrac{1}{2}m\left(\dot{r}^2 + (r\dot{\phi})^2\right) + \frac{e^2}{r}\,. \tag{5.61}$$

Thus we have two generalized momenta

$$p_r = \frac{\partial L}{\partial \dot{r}} = m\dot{r}\,, \qquad p_\phi = \frac{\partial L}{\partial \dot{\phi}} = mr^2\dot{\phi}\,, \tag{5.62}$$

and the Hamiltonian is

$$H = \frac{1}{2m}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right) - \frac{e^2}{r}\,. \tag{5.63}$$

For simplicity sake let us take a circular classical trajectory, hence $\dot{r} = 0$ and only only p_ϕ is different from zero. Thus the action (5.53) for this trajectory reduces to

$$\oint p\, dq = \int_0^T dt p_\phi\, \dot{\phi} = \int_{\phi_a}^{\phi_b} d\phi\, p_\phi\,. \tag{5.64}$$

Thus the quantization condition becomes

$$\oint d\phi\, p_\phi = 2\pi\hbar\,(n+1) = 2\pi\hbar\,\nu\,, \tag{5.65}$$

where $\nu = 1, 2, 3, \ldots$. From the Hamilton equations we eliminate r and express p_ϕ in terms of the energy

$$E = \frac{1}{2m}\left(p_r^2 + \frac{p_\phi^2}{r^2}\right) - \frac{e^2}{r}\,, \tag{5.66}$$

and obtain

$$p_\phi = \sqrt{-\frac{m}{2}\frac{e^4}{E}}\,. \tag{5.67}$$

Since p_ϕ does not depend on ϕ we obtain from (5.51)

$$E = -m\frac{e^4}{2\hbar^2}\frac{1}{\nu^2}\,, \qquad \nu = 1, 2, \ldots\,. \tag{5.68}$$

This is the well known Bohr's formula for the hydrogen spectrum.

One may wonder whether restricting the above calculations to a circular trajectory leads to oversimplified results. This is not so. One can do similar calculations to the above ones but for an arbitrary elliptic orbit and get the same results. Now the situation is somewhat more complicated: p_r is not zero, and we have two constants of motion which determine p_ϕ and p_r which in turn determine the l.h.s. of (5.53). Following (5.53) we have now two objects to quantize, p_ϕ and p_r. We have also two constants of motion to employ

$$p_\phi = M\,, \qquad \frac{1}{2m}\left(p_r^2 + \frac{M^2}{r^2}\right) - \frac{e^2}{r} = E\,. \tag{5.69}$$

Fixing $M \geq 0$ and $E < 0$ we fix the excentricity of the elliptic trajectory:

$$\epsilon^2 = 1 + \frac{M^2 E}{2me^4}\,. \tag{5.70}$$

So, now we have to have

$$\oint \sum_r p_r\, dq_r = \oint p_\phi\, d\phi + \oint p_r\, dr = 2\pi\hbar\nu\,, \qquad \nu = 1, 2, 3, \ldots\,. \tag{5.71}$$

Thus it is enough to make

$$\oint p_\phi d\phi = 2\pi\hbar l\,, \qquad \oint p_r dr = 2\pi\hbar k\,, \qquad \text{hence}\ \ \nu = l + k\,. \tag{5.72}$$

The first integral is easy ($p_\phi = const$):

$$M = l\hbar\,. \tag{5.73}$$

The second one is more complicated. We have to solve (5.69) for p_r, and integrate over r from $r = r_{\text{min}}$ to $r = r_{\text{max}}$ and back:

$$\oint p_r dr = 2\int_{r_{\text{min}}}^{r_{\text{max}}} p_r\, dr\,, \qquad p_r = \sqrt{2mE + 2m\frac{e^2}{r} - \frac{M^2}{r^2}}\,. \tag{5.74}$$

The minimal and maximal values of r one can get from the Kepler relation between r and the "true anomaly", $\Delta\phi$, i.e. the polar angle counted from the position of the perihelion (closest approach to the sun, here: to the hydrogen nucleus):

$$r = \frac{M^2}{2me^2(1+\epsilon\cos\Delta\phi)}\,. \tag{5.75}$$

After long but elementary calculations we get

$$\oint p_r\,dr = 2\pi k\hbar = \sqrt{\frac{2\pi^2 me^4}{-E}} - 2\pi M = 2\pi\hbar k\,. \tag{5.76}$$

Since $\nu = k + l$ we get again the Bohr formula

$$E_n = -\frac{me^4}{2\hbar^2\nu^2}\,. \tag{5.77}$$

5.3 The story of two actions

In (5.48) we defined the action S for a given time T. This relation taken as a Legendre transformation, see Appendix C, implicitely introduces the action $\tilde{S}$ defined for a given energy E. We can write $\tilde{S}$ in terms of integrals over time (q and p stand for the generalized coordinates and momenta):

$$\tilde{S}(b,a,E) = \int\limits_0^{T(E)} dt L(q,\dot{q}) + \int\limits_0^{T(E)} dt H(p,q) \tag{5.78}$$

or

$$S(b,a,T) = \tilde{S}(b,a,E) - ET\,, \tag{5.79}$$

where $T(E)$ is here the solution of the relation we have already encountered earlier

$$E = -\frac{\partial S(b,a,T)}{\partial T}\,. \tag{5.80}$$

Indeed, inserting

$$H(p,q) = \sum \dot{q}\frac{\partial L}{\partial \dot{q}} - L$$

into (5.78) we obtain

$$\tilde{S}(b,a,E) = \int_0^{T(E)} \sum p\dot{q}\,dt = \int_a^b \sum p\,dq\,. \tag{5.81}$$

Let us remind the reader that the action $\tilde{S}$ can also be employed to determine classical trajectories at fixed energy, E. One can find the equation of motion by adding a small deviation to the trajectory and demanding that the first variation of $\tilde{S}$ is zero: $\delta\tilde{S} = 0$. Note that now variations of the trajectory must keep $E = const$, thus are different from the ones we have been using thus far which keep $T = const$. In fact this was the first variational principle introduced into physics by Maupertuis [5.3] and Euler [5.4] in 1744–46.

In order to appreciate that S and $\tilde{S}$ are quite different let us calculate $\tilde{S}$ for a free particle with a given energy E, hence a constant momentum $p = \sqrt{2mE}$. From (5.81) we get

$$\tilde{S}_0 = |b-a|\sqrt{2mE}\,, \tag{5.82}$$

whereas

$$S_0 = \tfrac{1}{2}m\frac{(b-a)^2}{T}\,. \tag{5.83}$$

Let us extract now the energy levels of the system in the semiclassical approximation employing $\tilde{S}$. We start with the general formula for the Feynman propagator in the energy representation (given in (**??**)):

$$K(b,a,T) = \sum_n \phi_n(b)\,\phi_n^*(a)\,e^{-\frac{i}{\hbar}E_n T}\,,$$

where we suppressed the vector markings for the sake of simplicity. We take its Laplace transform

$$G(b,a,E) = \int_0^\infty dT K(b,a,T)\,e^{\frac{i}{\hbar}ET} = \sum_n \phi_n(b)\,\phi_n^*(a)\int_0^\infty dT\,e^{\frac{i}{\hbar}(E-E_n)T}\,. \tag{5.84}$$

The intergals over T are well defined when we give E a small positive imaginary part $E \to E + i\epsilon$. Then

$$G(b,a,E) = i\hbar\sum_n \frac{\phi_n(b)\,\phi_n^*(a)}{E+i\epsilon-E_n}\,. \tag{5.85}$$

Thus the poles of $G(b,a,E)$ give us the eigenvalues of the energy, and their residua are determined by the corresponding wave functions. Note that $G(b,a,E)$ satisfies the following equation (H_b being the Hamilton operator acting on the variable b):

$$(E-H_b)\,G(b,a,E) = i\hbar\sum_n \phi_n(b)\,\phi_n^*(a) = i\hbar\,\delta(b-a)\,. \tag{5.86}$$

Therefore, $G(b,a,E)$ is not a propagator but rather a Green's function. Note that the composition principle valid for the propagators

$$K(b,a,T) = \int dc\,K(b,c,T-t_c)\,K(c,a,t_c)\,, \tag{5.87}$$

where t_c is any moment inside the evolution time T ($0 < t_c < T$) is *not applicable* to the Green functions $G(b,a,E)$. More specifically the composition

$$\int dc\,G(b,c,E)\,G(c,a,E') \neq G(b,a,E)\,,$$

for whatever E, E' might be, is not a Green function any more. The energy E is not a variable which could control an evolution of a trajectory from a to b – in this case there is simply no evolution.

We apply this operation to the semiclassical propagators (5.44). We have to calculate (remember that the sum over τ runs over a set of *classical* trajectories, some examples are worked out below)

$$G_{sc}(\mathbf{b},\mathbf{a},E) = \sum_\tau \left(\frac{i}{2\pi\hbar}\right)^{\frac{3}{2}} e^{-in_\tau \frac{1}{2}\pi} \int_0^\infty dT \sqrt{\left|det\frac{\partial^2 S_\tau}{\partial\mathbf{a}\partial\mathbf{b}}\right|}\, e^{\frac{i}{\hbar}(ET+S_\tau(\mathbf{a},\mathbf{b},T))} \,. \tag{5.88}$$

This we do employing the stationary phase approximation to the integral over time (the factor $\sqrt{|det...|}$ we assume to be weakly depending on T, as compared to $\exp(i(ET...)/\hbar)$, and take it out of the integral). This is reasonable because, when $\hbar$ is small, the exponent oscillates violently and the dominant contribution comes from around the stationary point. Thus we seek the stationary point, $T_{\tau\sigma}$ (for each trajectory τ there may be more than one labelled by σ) solving the equation

$$\frac{\partial}{\partial T}(ET + S_\tau(b,a,T)) = E + \frac{\partial S_\tau(b,a,T)}{\partial T} = 0\,. \tag{5.89}$$

Note that the last part of (5.89) is the general relation (5.80) We expand the exponent of the integrand around the solution of (5.89)

$$T_{\tau\sigma} = T_{\tau\sigma}(b,a,E)\,, \tag{5.90}$$

and get

$$ET + S_\tau(b,a,T) \;\approx\; \tilde{S}_{\tau\sigma} + \frac{1}{2}\frac{\partial^2 S_\tau}{\partial T^2}\bigg|_{T_{\tau\sigma}} (T-T_{\tau\sigma})^2 + \dots\,, \tag{5.91}$$

where

$$\tilde{S}_{\tau\sigma}(b,a,E) = ET_{\tau\sigma} + S_\tau(b,a,T_{\tau\sigma}) \tag{5.92}$$

is an action integral which is also defined by a trajectory going from a to b but instead of a given time T the energy E is fixed. So, (5.88) becomes

$$G_{sc}(b,a,E) = \sum_\tau \left(\frac{i}{2\pi\hbar}\right)^{\frac{3}{2}} e^{-in_\tau\frac{1}{2}\pi + \frac{i}{\hbar}\tilde{S}_{\tau\sigma}} \sqrt{\left|det\frac{\partial^2 S_\tau}{\partial a\partial b}\right|} \int_0^\infty dT\, e^{\frac{i}{2\hbar}\frac{\partial^2 S_{\tau\sigma}}{\partial T^2}(T-T_{\tau\sigma})^2}\,.$$

Extending the integration over T from $-\infty$ to $+\infty$ we get

$$G_{sc}(b,a,E) = -\frac{1}{2\pi\hbar}\sum_{\tau\sigma}\sqrt{|D_{\tau\sigma}|}\, e^{-in_\tau\frac{1}{2}\pi + \frac{i}{\hbar}\tilde{S}_{\tau\sigma}}\,, \tag{5.93}$$

where

$$D_{\tau\sigma} \;=\; \frac{\det\left(\frac{\partial^2 S_{\tau\sigma}}{\partial a\partial b}\right)}{\frac{\partial^2 S_{\tau\sigma}}{\partial T^2}} \;=\; \frac{\partial^2 \tilde{S}_{\tau\sigma}}{\partial a\partial b}\frac{\partial^2 \tilde{S}_{\tau\sigma}}{\partial E^2} - \frac{\partial^2 \tilde{S}_{\tau\sigma}}{\partial a\partial E}\frac{\partial^2 \tilde{S}_{\tau\sigma}}{\partial b\partial E}\,. \tag{5.94}$$

A comment on our somewhat confusing notation is here in order. In one space dimension the symbol det(...) upstairs on l.h.s. is redundant (the determinant is just one number). On the r.h.s. however, we have a two dimensional determinant explicitly written down. In n dimensions we have a $n \times n$ determinant on the l.h.s.,and a $(n+1) \times (n+1)$ determinant on the r.h.s.. The n by n determinant constructed from the $n \times n$ derivatives of $\tilde{S}$ is supplemented by the column of n elements $\partial^2 \tilde{S}/\partial a_i \partial E$, and by a row of n elements $\partial^2 S/\partial E \partial b_i$.

Comparing (5.93) with (5.44) for the semiclassical propagator with fixed time T we see that $|D_{\tau\sigma}|$ in (5.93) is the analogue of $|\det \partial^2 S/\partial a \partial b|$ in (5.44) which gives the density of trajectories with fixed time T. Thus we accept that $|D_{\tau\sigma}|$ gives the density of trajectories on the energy surface fixed by E. eq.(5.94) provides us with a relation between these two densities. The last step in (5.94) one can obtain expressing the density of trajectories with fixed T through the action for fixed energy, E (we skip the subscripts for the sake of simplicity).

One more comment on (5.93) is in order: n_τ in the phase factor is the number of conjugate points but *now the conjugate points are determined by the singularities of $D_{\tau\sigma}$, hence by the density of trajectories at fixed E.*

To prove (5.94) we start with the relation (5.92). Differentiating it with respect to E, and then with respect to T we get two “sister” relations

$$\frac{\partial \tilde{S}(b,a,E)}{\partial E} = T\,, \qquad -\frac{\partial S(b,a,T)}{\partial T} = E\,. \tag{5.95}$$

Keeping T fixed, we differentiate the first one with respect to a. We get

$$\frac{\partial T}{\partial a} = \frac{\partial}{\partial a}\frac{\partial \tilde{S}}{\partial E} = \frac{\partial^2 \tilde{S}}{\partial a \partial E} + \frac{\partial^2 \tilde{S}}{\partial E^2}\frac{\partial E}{\partial a} = 0\,, \tag{5.96}$$

and the same for b. Thus we have

$$\frac{\partial E}{\partial a} = -\frac{\partial^2 \tilde{S}}{\partial E \partial a}\left(\frac{\partial^2 \tilde{S}}{\partial E^2}\right)^{-1}, \tag{5.97}$$

$$\frac{\partial E}{\partial b} = -\frac{\partial^2 \tilde{S}}{\partial E \partial b}\left(\frac{\partial^2 \tilde{S}}{\partial E^2}\right)^{-1}. \tag{5.98}$$

We write (5.92) in the form

$$S(b,a,T) \;=\; \tilde{S}(b,a,E(b,a,T)) - E(b,a,T)T\,. \tag{5.99}$$

Now a judicious differentiation of the above (remember that T is fixed and that $T = \partial \tilde{S}/\partial E$) gives

$$\frac{\partial^2 S}{\partial a \partial b} = \frac{\partial^2 \tilde{S}}{\partial a \partial b} + \frac{\partial^2 \tilde{S}}{\partial E \partial a}\frac{\partial E}{\partial b}\,. \tag{5.100}$$

Employing (5.95) we obtain

$$\frac{\partial^2 S}{\partial a \partial b} = \frac{\partial^2 \tilde{S}}{\partial a \partial b} - \frac{\partial^2 \tilde{S}}{\partial a \partial E}\frac{\partial^2 \tilde{S}}{\partial b \partial E}\left(\frac{\partial^2 \tilde{S}}{\partial E^2}\right)^{-1}. \tag{5.101}$$

On the other hand we have from the two relations (5.95), with a, b fixed this time

$$\delta E = -\frac{\partial^2 S}{\partial T^2}\,\delta T\,, \qquad \delta E = \left(\frac{\partial^2 \tilde{S}}{\partial E^2}\right)^{-1}\delta T\,. \tag{5.102}$$

Equating these two δE's we get

$$\left(\frac{\partial^2 S}{\partial T^2}\right)^{-1} = -\frac{\partial^2 \tilde{S}}{\partial E^2}\,. \tag{5.103}$$

Multiplying both sides of (5.101) by $\partial^2 S/\partial E^2$ and employing (5.103) we obtain (5.94).

From (5.102) we see that when we keep E fixed but let T vary $\partial^2 S/\partial T^2 = 0$, on the other hand, when we keep T fixed and vary E we have $\partial^2 S/\partial T^2 = \infty$. These are the places where the classical trajectories focus in these two cases. In other words where $\partial^2 S/\partial b\partial a$ hits a singularity (a conjugate point) we have also a singularity of $\partial^2 S/\partial T^2$, see example below.

Example: Semiclassical approximation for the harmonic oscillator

The action for the harmonic oscillator

$$S(b,a,T) = \frac{m\omega}{2\sin\omega T}\left[(a^2+b^2)\cos\omega T - 2ab\right], \tag{5.104}$$

gives

$$\frac{\partial^2 S}{\partial b\partial a} = -\frac{m\omega}{\sin\omega T}\,. \tag{5.105}$$

Therefore, where $\sin\omega T = 0$, $\partial^2 S/\partial b\partial a$ has a singularity and changes its sign. Thus the propagator $K(b,a,T)$ acquires the phase $\exp(-i\pi/2)$.

We calculate

$$E(b,a,T) = -\frac{\partial S(b,a,T)}{\partial T} = \frac{m\omega^2}{2}\frac{(a^2+b^2) - 2ab\cos\omega T}{\sin^2\omega T}\,, \tag{5.106}$$

and then

$$-\frac{\partial^2 S(b,a,T)}{\partial T^2} = \frac{\partial E}{\partial T} = m\omega^3\,\frac{2ab - ab\sin^2\omega T + (a^2+b^2)\cos\omega T}{\sin^3\omega T}\,. \tag{5.107}$$

Now we calculate D at the conjugate points ($\sin\omega T = 0$, $\cos\omega T = \pm 1$)

$$-\left.\frac{\partial^2 S/\partial b\partial a}{\partial^2 S/\partial T^2}\right|_{\left(\substack{\sin\omega T=0\\ \cos\omega T=\pm1}\right)} = \frac{m\omega\sin^2\omega T}{m\omega^3(2ab \pm (a^2+b^2))}\,, \tag{5.108}$$

where we left the factor $\sin\omega T$ to show that:

(a) the sigularities of $\partial^2 S/\partial b\partial a$ are cancelled by $\partial^2 S/\partial T^2$, and D is zero there,

(b) D goes through zero *but it does not change the sign.* Thus these points do not generate any phase factors.

Let us consider now the trajectories of fixed energy E.

$$E = \tfrac{1}{2}m\dot{x}^2 + \tfrac{1}{2}m\omega^2 x^2\,, \tag{5.109}$$

thus

$$\frac{dx}{dt} = \pm\sqrt{\frac{2}{m}(E - \tfrac{1}{2}m\omega^2 x^2)}\,, \tag{5.110}$$

where $\pm$ gives two possible directions of motion. Now we calculate the time T needed for the particle of a fixed energy E to go from a to b:

$$\begin{aligned} T &= \int_a^b \frac{dx\sqrt{m}}{\sqrt{2(E - \frac{1}{2}m\omega^2 x^2)}} = \frac{1}{\omega}\int_{a\sqrt{\frac{m\omega^2}{2E}}}^{b\sqrt{\frac{m\omega^2}{2E}}} \frac{du}{\sqrt{1-u^2}} \\ &= \frac{1}{\omega}\left[\arcsin b\sqrt{\frac{m\omega^2}{2E}} - \arcsin a\sqrt{\frac{m\omega^2}{2E}}\right], \end{aligned} \tag{5.111}$$

and then calculate

$$\frac{\partial T}{\partial E} = -\frac{1}{\partial^2 S/\partial T^2} = -\frac{1}{2}\sqrt{\frac{m}{2}}E^{-\frac{3}{2}}\left[\frac{b}{\sqrt{1-\frac{m\omega^2}{2E}b^2}} - \frac{a}{\sqrt{1-\frac{m\omega^2}{2E}a^2}}\right] \tag{5.112}$$

to find singularities of $G(b,a,E)$.

Now a few comments are in order. $\pm x_T = \pm\sqrt{2E/m\omega^2}$ are the two turning points where the particle stops and reverses its direction of motion. Hence we see that $G(b,a,E)$ goes through a singularity every time the particle is at $\pm x_T$. Let us suppose that our particle starts from a goes to the right, reaches x_T and slides down to b. Now the time it takes to go from a to b is the sum of two times: $T = T_1 + T_2$, where T_1 is for going from a to x_T, and T_2 for going from x_T to b,

$$T = T_1 + T_2 = \frac{1}{\omega}\left[\lim_{b\to x_T}\arcsin(\frac{b}{x_T}) - \arcsin(\frac{a}{x_T})\right] + \frac{1}{\omega}\left[\frac{\pi}{2} - \arcsin(\frac{b}{x_T})\right].$$

The singularity of $\partial T/\partial E$ *before* b reached x_T comes from the derivative with respect to E of

$$\arcsin\left(\frac{b}{x_T}\right),$$

whereas when b *has passed* x_T it comes from

$$-\arcsin\left(\frac{b}{x_T}\right).$$

Thus $\partial T/\partial E$ *changes sign every time it goes through* $\pm x_T$, and each such passage adds the factor $\exp(-i\pi/2)$. But, for a given (a,b), there are infinitely many classical trajectories of fixed E, and each of them is characterized by the number of passages through the turning points, n_τ, hence contributes the factor $\exp(-i\pi n_\tau/2)$. In $G_{sc}(b,a,E)$ we have to sum over all $\tau's$.

From the relation (5.117) below, one can get the spectrum of a system finding poles of $G(b,a,E)$. It can be done for $G_{sc}(b,a,E)$ after the sum over τ is performed. One can show [5.1] that for a partice moving in a potential

$V(x)$ which $V(\pm\infty) = +\infty$ we get the following factor in G_{sc} which exhibits singularities in E

$$G_{sc}(b,a,E) \sim \frac{1}{1 - \exp\left\{\frac{2i}{\hbar}\int_{x_T(L)}^{x_T(R)} dx\,\sqrt{2m(E-V(x)} - \hbar\pi\right\}}\,, \tag{5.113}$$

where $x_T(R)$ and $x_T(L)$ are the right and the left turning points, respectively. Thus $G_{sc}(b,a,E)$ has singularities at $E's$ which satisfy the following equation

$$1 = \exp\left\{\frac{2i}{\hbar}\int_{x_T(L)}^{x_T(R)} dx\,\sqrt{2m(E-V(x)} - \hbar\pi\right\}\,. \tag{5.114}$$

For the harmonic oscillator we have

$$2\int_{x_T(L)}^{x_T(R)} dx\,\sqrt{2m(E-V(x)} = 2\pi\frac{E}{\omega}\,, \tag{5.115}$$

hence we get the following condition for a singularity to occur

$$2\pi\,\frac{E}{\omega} = 2\pi\hbar\left(l+\tfrac{1}{2}\right)\,, \qquad l = 0,1,2,\ldots\,, \tag{5.116}$$

and we get the well known result: $E = \hbar\omega(l+\frac{1}{2})$.

End of Example

Extraction of the energy spectra from the propagators $K(b,a,T)$ or the Green functions $G(b,a,E)$ is one of the important applications of the method of path integrals. Above, we have applied the single valuedness of the propagators along a closed classical trajectory to obtain the energy spectra of some quantal systems. Now we shall briefly discuss the method taking traces of K or G for the same purposes.

First let us write K and G in the representation of energy eigenstates:

$$\begin{aligned} K(b,a,T) &= \sum_l \phi_l(b)\,\phi_l^*(a)\,e^{-\frac{i}{\hbar}E_lT}\,, \\ G(b,a,E) &= i\hbar\sum_l \frac{\phi_l(b)\,\phi_l^*(a)}{E-E_l+i\epsilon}\,. \end{aligned} \tag{5.117}$$

Their traces

$$\begin{aligned} \mathrm{Tr}\,K(b,a,T) &= \int dx\,K(x,x,T) = \sum_l e^{-\frac{i}{\hbar}E_lT}\,, \\ \mathrm{Tr}\,G(b,a,E) &= \int dx\,G(x,x,E) = i\hbar\sum_l \frac{1}{E-E_l+i\epsilon} \end{aligned} \tag{5.118}$$

depend only on the energy eigenvalues (and the constants of trajectories T or E).

Let us look at the example of the harmonic oscillator

$$
\begin{aligned}
\operatorname{Tr} K(b,a,T) &= \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} \int\limits_{-\infty}^{+\infty} dx\, e^{\frac{i}{\hbar}\frac{m\omega}{2\sin\omega T}(2x^2\cos\omega T - 2x^2)} \\
&= \left(\frac{m\omega}{2\pi i\hbar \sin\omega T}\right)^{\frac{1}{2}} \int\limits_{-\infty}^{+\infty} dx\, e^{-[\frac{i}{\hbar}2\frac{m\omega}{\sin\omega T}\sin^2\frac{\omega T}{2}]x^2} = \frac{1}{\sqrt{-1}}\frac{1}{2\sin\frac{\omega T}{2}} \\
&= \frac{1}{e^{i\frac{\omega T}{2}}(1-e^{-i\omega T})} = e^{-i\frac{\omega T}{2}} \sum_{l=0}^{\infty} e^{-il\omega T} = \sum_{l=0}^{\infty} e^{-(l+\frac{1}{2})\omega T}\,.
\end{aligned}
$$

Thus from (5.118) we obtain

$$
E_l \;=\; \left(l+\tfrac{1}{2}\right)\hbar\omega\,. \tag{5.119}
$$

This was an exact result, but when we have a potential with just one smooth minimum we can approximate it by a parabola and, in the semiclassical approximation, we have a harmonic oscillator again. Indeed,

$$
L \;=\; \tfrac{1}{2}m\dot{x}^2 - V(x) \;\approx\; \tfrac{1}{2}m\dot{x}^2 - V(\bar{x}) - \tfrac{1}{2}\left.\frac{d^2V}{dx^2}\right|_{x=\bar{x}} (\bar{x}-x)^2 + \ldots\,, \tag{5.120}
$$

where at $\bar{x}$ the potential $V(x)$ has its minimum, $dV/dx|_{x=\bar{x}} = 0$. We build the semiclassical propagator around the trajectory $x(t) = \bar{x} = \text{const}$:

$$
K(b,a,T) \;=\; e^{\frac{i}{\hbar}S[\bar{x}]} \int [\mathcal{D}y(t)]\, e^{\frac{i}{\hbar}\int_0^T dt\,(\frac{1}{2}m\dot{y}^2 - \frac{1}{2}\frac{d^2V}{dx^2}\big|_{\bar{x}}y^2)}\,. \tag{5.121}
$$

Since $S[\bar{x}] = -V(\bar{x})T$, and we can define the constant

$$
\left.\frac{d^2V}{dx^2}\right|_{\bar{x}} \;=\; m\omega^2\,, \tag{5.122}
$$

we find

$$
\operatorname{Tr} K(b,a,T) = e^{-\frac{i}{\hbar}V(\bar{x})T} \sum_l e^{-\frac{i}{\hbar}(l+\frac{1}{2})\hbar\omega T}\,. \tag{5.123}
$$

Thus, in the semiclassical approximation, we have

$$
E_l \;\approx\; V(\bar{x}) + (l+\frac{1}{2})\hbar\omega\,. \tag{5.124}
$$

We close this section with the following general comment. Into a mathematical analysis of the traces $\operatorname{Tr} T$ and $\operatorname{Tr} G$ an impressive intellectual effort has been invested (a comprehensible discussion of these and related problems one finds in ref. [5.6]). In particular $\operatorname{Tr} G(E)$ can be cast in the form of the *trace formula* [5.6] which is a sum over contributions from periodic orbits and is able to give the spectral structure of some chaotic systems. The special role of periodic orbits seems to fulfill the prophecy of Poincare:

"...what makes these periodic solutions so valuable, is that they offer in a manner of speaking, the only opening through which we might try to penetrate into the fortress which has the reputation of being impregnable".

Appendix C: The Legendre transformation

Let $f(x,y)$ be a function of two variables x, y:

$$df = udx + vdy\,, \qquad u = \frac{\partial f}{\partial x}\,, \qquad v = \frac{\partial f}{\partial y}\,. \tag{C.1}$$

Suppose we want to change the basic variables from x, y to u, in the function g defined as follows:

$$g = f - \frac{\partial f}{\partial x}x = f - ux\,. \tag{C.2}$$

Also

$$dg = df - udx - xdu = vdy - xdu\,. \tag{C.3}$$

The quantities v, x are now $v = \partial g/\partial y$, $x = -\partial g/\partial u$. We can get

$$g(y,u) = f - ux \tag{C.4}$$

by solving $u = \partial f(x,y)/\partial x$ for $x = x(u,y)$ and inserting this x into (C.4). We can also write

$$dg = \frac{\partial g}{\partial y}dy - \frac{\partial g}{\partial u}du\,. \tag{C.5}$$

The relations between H and L, and between S and $\tilde{S}$ are thus Legendre transformations.

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