Chapter 1

Introduction and a disclaimer

The purpose of these set of lectures is to introduce the field of semiclassical mechanics and illustrate the principle of classical-quantum correspondence. It is difficult to do justice to the subject in just ten lectures - given the range and depth of the topic this would mean one lecture for every decade of progress. Moreover, I do not think that I have the required maturity to talk on a subject which, in my personal opinion, is exceptionally beautiful. In this regard there are far better people than me to do the job. I do, however, have one qualification which is that of an untiring enthusiasm for understanding the link between the classical and the quantum world. Sometimes the enthusiasm borders on, what might seem like, fanaticism but I take solace from the following words of Boltzmann in his address to the meeting of natural scientists in Munich in 1899:

“I therefore present myself to you as a reactionary, one who has stayed behind and remains enthusiastic for the old classical doctrines as against the men of today; but I do not believe that I am narrow-minded or blind to the advantages of the new doctrines, which shall receive due justice in the next section of my talk, so far as lies within my power; for I am well aware that like everyone else, I see things subjectively tinged through my own spectacles”

1.1 Historical comments and motivations

In this introductory lecture I would like to motivate the subject with some key comments made by the creators of quantum mechanics. The point of highlighting these comments is to emphasize the crucial role played by classical mechanics in the development of quantum mechanics. By crucial role, I do not mean only the spectacular failures of classical mechanics, as described in many textbooks, but more to do with the close parallels that motivated
people like Heisenberg, Dirac, Schrödinger, Born, and many others. For example, in Heisenberg’s paper, every formula of quantum mechanics is motivated by a corresponding classical formula. As soon as one mentions the word ‘correspondence’ the name Niels Bohr immediately comes to mind. It would not be wrong to say that the correspondence principle of Bohr is the starting point for a century of debate and work on classical-quantum correspondence. Although the ideas in the seminal 1913 paper of Bohr have been largely overshadowed by the modern quantum mechanics that we all learn, it is instructive to hear as to what Einstein had to say:

“That this insecure and contradictory foundation was sufficient to enable a man of Bohr’s unique instinct and perceptiveness to discover the major laws of the spectral lines and of the electron shells of the atom as well as their significance for chemistry appeared to me like a miracle and appears as a miracle even today. This is the highest form of musicality in the sphere of thought.”

The central aspect of correspondence principle is that somehow in the limit of large quantum numbers, the new quantum mechanics must ‘reduce’ to the old classical mechanics. Indeed much of the early pioneering work in quantum theory was intimately tied to the correspondence philosophy of Bohr. For instance, J. H. Van Vleck in his 1924 paper on the relation between absorption of radiation by multiply periodic orbits and the correspondence principle says:

“One particular term in the classical radiation force is thus competent to bring an orbit from one stationary state to another...... It is proved that for large quantum numbers the classical theory value for the ratio of absorption to emission approaches asymptotically the quantum theory expression for the ratio of the differential absorption to the spontaneous emission.”

Note that I have highlighted the word ‘asymptotically’ since that single word captures the quantum to classical transition process in a fairly accurate manner. In the later lectures we will see that Van Vleck made a seminal contribution to semiclassical mechanics which is the cornerstone for many of the recent applications in chemical dynamics. As another example consider the following opening paragraph from the famous 1916 paper of Ehrenfest on adiabatic invariants

“In the treatment of a continually increasing number of physical problems, use is at the same time made of the principles of classical mechanics and electrodynamics, and of the hypothesis of the quanta, which is in conflict with them. Through the study of these problems it is hoped to arrive at some
general point of view which may trace the boundary between the ‘classical region’ and the ‘region of the quanta’.

As an example of the classical-quantum correspondence, consider the question: Is there a relation between the orbital motion of the electron in an atom and the properties of light emitted by the atom? There is no reason to expect such a connection between the optical and orbital frequencies - we now know that energy levels are discrete and optical frequencies correspond to transitions between the discrete quantum levels i.e., quantum jumps. But suppose we consider the optical transition frequency in a hydrogen atom

$$\omega_{nm} = K \left( \frac{1}{m^2} - \frac{1}{n^2} \right)$$  \hspace{1cm} (1.1)

For the transitions from \( n = 5 \) to \( m = 4, 3, 2, 1 \) involving small quantum numbers the relative frequencies are \( \omega \equiv \omega_{5,4}, 3.2\omega, 9.3\omega, \) and \( 43\omega \) respectively. On the other hand if we look at transitions involving large quantum numbers e.g., from \( n = 500 \) to \( m = 499, 498, 497, 496 \) we find the frequencies \( \omega \equiv \omega_{500,499}, 2.0\omega, 3.0\omega, \) and \( 4.0\omega \) respectively. In other words, for transitions involving large quantum numbers (highly excited states) one gets a harmonic spectrum. It is the same frequencies that one would obtain if we write the classical periodic motion of the electron as a Fourier series

$$x(t) = a_1 \cos \omega t + a_2 \cos 2\omega t + \ldots$$  \hspace{1cm} (1.2)

Therefore in this large quantum number limit there is an intimate connection between the quantum jumps and the underlying periodic classical motion of the electron. At this point of time it is useful to mention that, contrary to the presentation in texts, Bohr’s 1913 paper did not start out with the quantization of angular momentum ansatz - that came later and naturally as a consequence of the following semiclassical statement: light that induces transitions between two states should have a frequency that is the arithmetic mean of the actual rotational frequencies of the electrons in the two states. Let us apply this to an electron on a ring. According to Bohr’s rule, and using the Planck-Einstein condition \( E = h\nu \),

$$h\nu \equiv h\omega = \hbar \left( \frac{\omega_f + \omega_i}{2} \right) = \frac{I}{2} \left( \omega_f^2 - \omega_i^2 \right)$$  \hspace{1cm} (1.3)

with \( I \) being the moment of inertia and \( \omega_f, \omega_i \) being the circular frequencies of the final and initial states. Starting with an initial state that is frozen i.e., zero angular momentum we get \( \omega_f = \hbar/I \) and thus the first excited state has kinetic energy \( I\omega_i^2/2 = \hbar^2/2I \). The corresponding transition frequency \( \omega = \hbar/2I \). Suppose we now start with the first excited state \( \omega_i = \hbar/I \).
Then the second excited state has $\omega_f = 2\hbar / I$ and the transition frequency $\omega = 3\hbar / 2I$. One can go on in this fashion and discover the energy levels of the standard particle on a ring problem in quantum mechanics.

Incidentally, such quantum-classical analogies are central to the formulation of Heisenberg’s matrix mechanics. It is interesting to note that the title of Heisenberg’s paper is “Quantum-theoretical re-interpretation of kinematic and mechanical relations”. Kinematics is the study and description of motion without regard to its causes (dynamics). So, Heisenberg assumed that the equations of motion of an electron can be retained but the kinematic interpretation of $x(t)$ as a location depending on time has to be rejected. This is further emphasized by Dirac’s 1926 paper on the fundamental equations of quantum mechanics wherein he states that:

“In a recent paper Heisenberg puts forward a new theory which suggests that it is not the equation of classical mechanics that are in any way at fault, but that the mathematical operations by which physical results are deduced from them require modification. All the information supplied by the classical theory can thus be made use of in the new theory.”

I have stressed upon the last sentence of Dirac’s since it is the heart and soul of all semiclassicalists! A judicious mix of classical and quantum mechanics should yield valuable insights into the behaviour of the system. This paper of Dirac is a must read for all beginning students of quantum mechanics. In particular, Dirac establishes the fundamental semiclassical result

$$\frac{1}{i\hbar} [\hat{x}, \hat{y}] \sim \{x, y\} + O(\hbar) \quad (1.4)$$

which states that the difference between the Heisenberg products (the quantum commutator on the left hand side above) asymptotically corresponds to the classical Poisson bracket $\{x, y\}$ involving the same variables. Later we will see the contributions and generalizations along these lines due to Weyl, Wigner, Moyal, and others.

This introductory lecture would be incomplete without quoting a supremely semiclassical viewpoint by Schrödinger: *The Hamiltonian analogy of mechanics to optics is an analogy to geometrical optics, since to the path of the representative point in configuration space there corresponds on the optical side the light ray, which is only rigorously defined in terms of geometrical optics. The undulatory elaboration of the optical picture leads to the surrender of the idea of the path of the system, as soon as the dimensions of the path are not great in comparison with the wave-length. Only when they are so does the idea of the path remain, and with it classical mechanics as an approximation; whereas for “micro-mechanical” motions the fundamental equations
of mechanics are just as useless as geometrical optics is for the treatment of diffraction problems. In analogy with the latter case, a wave equation in configuration space must replace the fundamental equations of mechanics (Abstract, Collected papers on wave mechanics, 1928).

There are many other studies early on which rely on the classical-quantum correspondence and deal with the asymptotic limit $\hbar \to 0$. Understanding this limit is of great fundamental importance but the story is not yet complete. The main stumbling block has to do with the fact that classical mechanics can exhibit both regular and irregular (chaotic) motion. Perhaps the first recognition of the extremely complicated nature of chaotic motion was made by Poincaré who says:

“If one seeks to visualize the pattern formed by these two curves and their infinite number of intersections, each corresponding to a doubly asymptotic solution, these intersections form a kind of lattice-work, a weave, a chain-link network of infinitely fine mesh; each of the two curves can never cross itself, but it must fold back on itself in a very complicated way so as to recross all the chain-links an infinite number of times.

One will be struck by the complexity of this figure, which I am not even attempting to draw. Nothing can give us a better idea of the intricacy of the three-body problem, and all of the problems of dynamics in general, when there is no uniform integral and the Bohlin series diverge.”

Now, if one needs a clean interpretation of the way quantum mechanics reduces to classical mechanics then it is crucial to answer the question: **What are the quantum manifestations of classical chaos?** In other words, if the classical-quantum bridge is to be built along the following scheme

$$\text{Quantum object} \sim \text{Classical object} + O(\hbar) \quad (1.5)$$

then does chaos play spoilsport? Even before the issue of chaos, already there is a warning in the statement by Schrödinger above when he mentions the word “diffraction”. In the quantum context, the analogy to optical diffraction is the phenomenon of tunneling. Since there is no tunneling in classical mechanics, at least in the real time version of it, it would seem like semiclassics is doomed. Moreover tunneling observables behave like $\exp(-1/\hbar)$ and so trying for an algebraic correction as above seems to be a useless exercise. However, it is possible to develop a semiclassical theory for tunneling as well and I will attempt to give some account of this in the lectures.

But now, let me get back to the issue of chaos. In the above scheme, a quantum object could be an observable or a general operator and its matrix elements. The fundamental object is the wavefunction - what does that...
correspond to in the classical world? Surely, it cannot be a single classical trajectory since the uncertainty principle would not allow that. Turns out that it is a family of trajectories in the classical phase space. But, which family? Are there any constraints? What about interference effects? The answers depend on the nature of the classical dynamics - regular or chaotic. In the case that classical mechanics is completely regular \( i.e., \) integrable, it turns out that one can use the regular trajectories to construct a quantum wavefunction. In fact, the old quantum theory quantization condition of Bohr-Sommerfeld-Epstein

\[
\oint p_k dq_k = n_k \hbar \quad ; \quad k = 1, 2, \ldots, f
\]  

(1.6)

for a system with \( f \) degrees of freedom gives a partial answer. For instance, going back to the electron on a ring example of Bohr, the above condition becomes

\[
\int_0^{2\pi} (m\omega r)(rd\phi) \equiv \int_0^{2\pi} I\omega d\phi = 2\pi I\omega = nh
\]  

(1.7)

which is the angular momentum quantization condition. The integers \( n_k \) are interpreted as quantum numbers and thus the formula is semiclassical in nature - classical mechanics on the left and quantum mechanics on the right! However, for the above formula to hold one has to make a more severe (and restrictive) assumption: \textbf{separability of the degrees of freedom}. Integrability is a weaker condition \( i.e., \) separability implies integrability but the converse is not true. The correct answer came from Einstein in 1917! Here is Einstein:

\begin{quote}
"Notwithstanding the great successes that have been achieved by the Sommerfeld-Epstein extension of the quantum theory for systems of several degrees of freedom, it still remains unsatisfying that one has to depend on the separation of variables...because it probably has nothing to do with the quantum problem per se...the individual products \( dp_i dq_i \) in a system of several degrees of freedom...are not invariants, therefore the quantization condition has no invariant meaning."
\end{quote}

And then he made a “small modification”, based on Poincaré’s remark in 1911 that \( \sum p_i dq_i \) is invariant under coordinate transformations, to the quantization rule obtaining

\[
\oint_{C_k} \sum_{i=1}^f p_i dq_i \equiv \oint_{C_k} \mathbf{p} \cdot d\mathbf{q} = n_k \hbar
\]  

(1.8)

The quantities \( C_1, \ldots, C_f \) are \( f \) independent closed loops of a \( f \)-dimensional torus in the \( 2f \)-dimensional phase space. Amazingly enough, this paper of
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Einstein was ignored for nearly twentyfive years before being independently discovered by Keller in 1958. Now this coordinate-independent formulation is called as the Einstein-Brillouin-Keller (EBK) quantization. Even more impressive was the parting remark of Einstein in the 1917 paper that got straight to the heart of quantum chaos:

“If there exist fewer than \( f \) constants of motion, as is the case, for example, according to Poincaré in the three body problem, then the \( p_i \) are not expressible by the \( q_i \) and the quantum condition of Sommerfeld-Epstein fails also in the slightly generalized form that has been given here.”

This remark of Einstein was lost for nearly fifty years! In 1967 Gutzwiller made the key breakthrough - when the classical system is completely chaotic and all order is seemingly lost, the quantum mechanics latches on to the only remaining phase space objects - the periodic orbits.

Note that there are two takes on the semiclassical research. One is primarily concerned with details of the correspondence and explores things at a very fundamental level. Clearly, systems with a few degrees of freedom are the only ones that are amenable to this first take. The second one is to go ahead and apply semiclassical approximation to molecular systems - small and large. Here one is not bothered too much about the implications of chaos etc. Chaos is important, and so are the other phase space structures, but it is crucial to see as to how far one can stretch things. Afterall the promise of semiclassical methods is in their easy applicability to very large systems - precisely those for which quantum methods are prohibitively difficult. Nevertheless, both approaches are important. For example, the fundamental progress provides us with very neat and clever tricks to simplify the large system computations.

It is tempting to provide a glimpse of the progress made during the last few decades. However, due to time and space limits, I will now jump ahead and start with the lecture on semiclassical mechanics. A brief intro to classical mechanics is, however, necessary. Later lectures (last 3 or so) will highlight some of the key applications of semiclassical mechanics to chemical dynamics.
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Chapter 2

Semiclassical Mechanics

Quantum mechanical calculations, with due respect to the recent advances, are still difficult from a computational point of view and then there is the issue of insights. But we know that computing classical trajectories is relatively easy for multidimensional systems as compared to doing Quantum Mechanics and so, somehow we have to come up with a way which preserves the attractive aspects of classical mechanics without sacrificing the interference effects which are the hallmark of the quantum world (or, is it really?). This way, this technique or more properly this subject is called as Semiclassical Mechanics. In semiclassical mechanics we retain all the attractive features of classical mechanics and also have interference effects! So, how do we get interference effects? For this we boldly posit that each classical trajectory carries with it an amplitude and phase! This is not such an outrageous statement since Huygens’ theory of light waves (proposed long before quantum mechanics in 17th century) has the germs of this idea. What are these amplitudes and phases that one associates with a classical trajectory and how does one go about determining them and many other such questions start bubbling up at this juncture.

A direct clue comes from Dirac’s (who else) suggestion in an 1933 paper which culminated in Feynman’s celebrated Path Integrals. Indirect (not really but for the angle I am going to take for this article), but classic\(^1\), route involves what is now known as the (J)WKB (Jeffreys, Wentzel, Kramers Brillouin) theory. The WKB theory was introduced as a technique to solve the Schrödinger equation to some “approximate power of the Planck’s constant $\hbar$” and the accuracy depended upon how the potential varies with position etc (more about this later on). Both the Path Integral and WKB approach

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\(^1\)It is possible that Dirac being such a master of quantum-classical correspondence and being aware of the classic works of Bohr, Sommerfeld, Einstein and many others could have been led to such a suggestion but I am not very sure about this.
give the same answer\textsuperscript{2} which is not surprising since Feynman’s theory was an alternative derivation of the laws of Quantum mechanics. Now, what was this wonderfull suggestion of Dirac? Let me just state it cryptically for now,

\[
\langle b|a \rangle \overset{\hbar \rightarrow 0}{\sim} e^{iS[b,a]/\hbar},
\]

where we have used the Dirac Bra-Ket notation, \( b \) and \( a \) stand for some final and initial states of the quantum system and \( S[b,a] \) denotes the action.

Ok, now we have to worry about what this equation really means - you see, on one side we have a full blown quantum mechanical transition amplitude and on the other side (of the asymptotic relation) the exponential of some kind of an action (infact, the classical action!). This relation is only true as \( \hbar \rightarrow 0 \) and not at \( \hbar = 0 \). There is a world of difference here and lot of subtelties. To start off, \( \hbar \) is an universal, dimensionfull constant and so clearly it cannot go to zero and what this is really shorthand for is the statement that \textit{in this theory or system all the relevant actions are much greater than} \( \hbar \). The second point is that the right hand side of the above suggestion makes no sense at \( \hbar = 0 \) (mathematicians would say that there is an \textit{essential singularity} at \( \hbar = 0 \)). So, this limit that Dirac indicates is really a semiclassical limit i.e., somewhere between classical and quantum lands. When we said previously that attached with each classical trajectory is an amplitude and phase we meant it in a semiclassical sense. It is known that the absolute magnitude square of the transition amplitude is the probability and you also know that the wavefunction is a kind of amplitude. This means Dirac is saying that somehow in the semiclassical limit the wavefunction can be built out of a \textit{family of classical trajectories with phases attached to them which are the actions}.

Let us slow down here for a moment and think hard about why we need a family of classical trajectories to construct a quantum wavefunction and one trajectory won’t do! I will try to give two arguments and perhaps more can be given but these arguments can be stated without getting into too many intricacies. Firstly, I assume you are aware of the concept of a \textit{wavepacket} - Schrodinger and others and many others lately wanted to construct an object out of the quantum wavefunctions which would mimic classical mechanics as far as possible. What they constructed was a wavepacket. It turns out that it is the closest one can get to classical world from the quantum world and basically the centre of the wavepacket pretty much moves according to the classical equations of motion. The way they constructed the wavepacket was by taking combinations of many wavefunctions and so to mimic classical mechanics...
mechanics they needed not one wavefunction but many. Now, what we are trying to do is to mimic quantum mechanics by using classical objects and it is but natural\(^3\) that we would need more than one classical trajectory. In fact the analogy is a bit more strong but enough for now. The second argument has to do with phase space in classical mechanics. The dimensions of phase space are basically that of action which has the same dimensions as that of the Planck’s constant \(\hbar\). Now, in classical mechanics I can pick an initial condition with arbitrary precision in both position and momentum which is a violation as far as quantum mechanics is concerned because of the Heisenberg uncertainty principle. Infact according to the uncertainty principle, any intial condition in a cell of area \(\hbar\) is “smoothed over ” by quantum mechanics\(^4\). So, all the classical trajectories in that little cell of area \(\hbar\) are in some sense equally important or unimportant! Hence, more than one classical trajectory is needed to mimic quantum phenomena via semiclassical mechanics.

I just stated the Dirac suggestion in a cryptic way and now we will go through some digression (necessarily mathematical and hence the symbol at the start) to see the origins of Dirac’s suggestion by adopting the Path Integral perspective. So, we will do a very basic but important calculation and close the circle of ideas, although in a reverse way.

As I said before, in quantum mechanics the most important object is the transition amplitude for a system to go from some state at time \(t\) to some other state at time \(t'\). The absolute square of this transition amplitude tells us about the probability for such an event ot take place. For the sake of simplicity, let us consider a one degree of freedom quantum system described by the pair of conjugate operators \(Q\) and \(P\) satisfying
\[
[Q, P] = i\hbar .
\] (2.2)
The Hamiltonian operator is given as:
\[
H = \frac{1}{2m}P^2 + V(Q).
\] (2.3)

Let us denote the states of the system by \(|a\rangle\), \(|b\rangle\),... where we have adopted the Dirac Bra-Ket notation. The transition amplitude we are interested in is then given by
\[
\langle b(t')|a(t)\rangle = \langle b|\exp\left[-\frac{iH(t-t')}{\hbar}\right]|a\rangle \equiv K[b, t'; a, t],
\] (2.4)

\(^3\)I should warn you that I have not seen this argument before and I am invoking the symmetry gods with some kind of duality in mind and trepidation in heart!

\(^4\)Note that there is no quantum phase space and quite a few researchers are working on this to see if they can define one and if so what advantages one gains by doing so.
where we have used the fact that the Hamiltonian operator is the generator of time translations. Note that we are basically asking the amplitude for the process in which the quantum system, in state $|a\rangle$ at time $t$, makes a transition to (or will be found in) state $|b\rangle$ at time $t'$. Now, the first step in Feynman’s path integrals idea is to insert a complete set of position eigenstates giving us the following expression,

$$K[b, t'; a, t] = \int dq_1 dq_2 \langle b|q_2\rangle \langle q_2|\exp\left[-\frac{iH(t-t')}{\hbar}\right]|q_1\rangle\langle q_1|a\rangle. \quad (2.5)$$

By the laws of Bra-Ket, the overlaps $\langle b|q_2\rangle$ and $\langle q_1|a\rangle$ are just the regular old wavefunctions in position representation which can be denoted as $b^*(q_2)$ and $a(q_1)$ respectively. The object sandwiched between the two wavefunctions is called as the propagator and has central importance not only in path integrals but also rigorous semiclassical theories. To get some ideas about this propagator, we investigate the short time limit of an object

$$\langle q_2(t + \Delta t)|q_1(t)\rangle \approx \langle q_2| \exp\left[-\frac{iH\Delta t}{\hbar}\right]|q_1\rangle, \quad (2.6)$$

where, $\Delta t$ is supposed to be small$^5$. Now, for starters we can clearly write,

$$\langle q_2(t + \Delta t)|q_1(t)\rangle \stackrel{\Delta t \to 0}{\sim} \delta(q_2 - q_1), \quad (2.7)$$

where, $\delta(q_2 - q_1)$ is the Dirac delta “function”. For $\Delta t$ being very small, we can write approximately

$$\exp\left[-\frac{iH\Delta t}{\hbar}\right] \approx \exp\left[-\frac{iP^2\Delta t}{2m\hbar}\right] \exp\left[-\frac{iV(Q)\Delta t}{\hbar}\right], \quad (2.8)$$

with the error being of the order $(\Delta t)^2$ and the coefficients of the error terms involving the commutators of the momentum with the position.

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$^5$This is the basic object that one deals with in Path integrals which comes about by slicing the time $(t - t')$ into small short intervals.

- Why is the above an approximation? Work out to second order in $\Delta t$ the form of the error.
With such sufficiently short $\Delta t$ the potential $V$ does not vary too much in the neighbourhood of $q_1$ and $q_2$ and thus we can write

$$\langle q_2(t + \Delta t)|q_1(t)\rangle \approx \exp \left[\frac{-iV(q_1)\Delta t}{\hbar}\right] \langle q_2| \exp \left[\frac{-iP^2\Delta t}{2m\hbar}\right] |q_1\rangle. \quad (2.9)$$

The trick now is to insert a complete set of momentum states in the propagator on the right and realising that

$$\langle q|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp \left[\frac{ipq}{\hbar}\right], \quad (2.10)$$

one can show that,

$$\langle q_2(t + \Delta t)|q_1(t)\rangle \approx \left(\frac{me^{-i\pi/2}}{2\pi\hbar}\right)^{1/2} \exp \left[\frac{i}{\hbar} \left(\frac{m(q_2 - q_1)^2}{2\Delta t} - V(q_1)\Delta t\right)\right]. \quad (2.11)$$

- Show the above result. You will have to do a gaussian integral in momentum.

So, what we have here is a short time approximate propagator. One thing to note, and this is crucial, is that the exponent on the right hand side seems very much like a Lagrangian times $\Delta t$! That is more like an action and in fact it is easy to show that the exponent can be written as an action (short time)

$$S[2, 1; \Delta t] \equiv \int_{t}^{t+\Delta t} \mathcal{L}(q, \dot{q})dt', \quad (2.12)$$

since the potential is pretty much constant in that short time interval. In fact the first term in the exponent is the action for the free particle (classical action). So, putting it all together we have

$$\langle q_2(t + \Delta t)|q_1(t)\rangle \approx \left(\frac{me^{-i\pi/2}}{2\pi\hbar}\right)^{1/2} \exp \frac{i}{\hbar} S[2, 1; \Delta t], \quad (2.13)$$

and there we have the haze of Dirac’s idea! For now also note that the prefactor (amplitude) can be related to some derivative of the action. All this from classical action!
2.1 The WKB approach

Now, one can continue along this line of thought and develop the full path integral idea and connect up to the semiclassical ideas by performing stationary phase trick. But let me take this opportunity to instead take a bit more of a traditional route leading up to the WKB results. We definitely are well motivated at this stage to try to solve the Schrodinger equation by using the following form of substitution:

\[ \psi(x, t) = \exp \frac{i}{\hbar} W(x, t), \quad (2.14) \]

where, \( W(x, t) \) is something to be specified and we are considering the solution of the time dependent equation. We will work in one dimension but the formal procedure can be easily written down in multidimensions. For now, one can think of this as a fancy change of variables and the resulting equation is

\[ -\frac{i\hbar}{2m} W_{xx}(x, t) + \frac{1}{2m} W_x^2(x, t) + V(x) = -W_t(x, t), \quad (2.15) \]

with the subscripts denoting the kind and order of differentials of the function \( W(x,t) \). It is important to note that we started with a linear equation and have turned it, by our substitution, into a nonlinear equation! This is typical of semiclassical methods in general and one might legitimately ask as to the usefulness of doing so - afterall, linear equations are easier to solve than the nonlinear ones. Let us not get into the details of this question here but just mention that the very basic classical equation is nonlinear and we are trying to build a bridge between classical and quantum mechanics. At this point we expand \( W(x,t) \) as a power series in \( \hbar \)

\[ W(x, t) = W_0(x, t) + \left( \frac{\hbar}{i} \right) W_1(x, t) + \left( \frac{\hbar}{i} \right)^2 W_2(x, t) + \ldots, \quad (2.16) \]

and note that the power series is usually not convergent but only asymptotic. Substituting the series into the transformed version of the time dependent Schrodinger equation and comparing we get equations at different orders of \( \hbar \). At the zeroth order i.e., \( O(\hbar^0) \) we have

\[ \frac{1}{2m} W_{0,xx}(x, t) + V(x) = -W_{0,t}(x, t), \quad (2.17) \]

which is nothing but the Hamilton-Jacobi equation of classical mechanics! This equation is of central importance in classical mechanics and it would
take a bit too long to expound all the beautifull aspects of this theory in this introduction (in addition to the fact that I am nowhere near qualified to do such a thing either!). Most of the so called good classical mechanics books, unfortunately, do a rather bad job of this topic. If you are interested, there are certain books you can look up to without fear of getting it all wrong. We will say a few things about it a bit later on down the road. Coming back to our series expansion at the next order, $O(\hbar^1)$, we have the equation

$$\frac{1}{2m} W_{0,x}^2(x,t) + \frac{1}{m} W_{0,x}(x,t) W_{1,x}(x,t) + W_{1,t}(x,t) = 0,$$

which is known as the amplitude transport equation. This is also a crucial equation as it can be rewritten in the form of an continuity equation for $|\psi(x,t)|^2$.

- Use the power series and the time dependent Schrodinger equation to show the above results.

It is clear from the above equations that we are going to get a hierarchy of equations at each order of $\hbar$ and that to solve an equation at some $O(\hbar^{k+1})$ we need to know the solutions of the initial equations up to $O(\hbar^k)$. It is customary to keep things only upto $O(\hbar)$ as there is no guarantee that things will converge as you go to higher orders. This, thus, leads to our approximate solution for the quantum equation,

$$\psi(x,t) \sim A(x,t) \exp \frac{i}{\hbar} S(x,t) + O(\hbar),$$

where, we have identified $W_0$ and $exp W_1$ with $S$ and $A$ respectively. The $S(x,t)$ represents the classical action and $A(x,t)$ denotes the amplitude - both classical objects. The equation above is an asymptotic relation. It is fairly easy to see at this stage that the quantum mechanical probability density is simply given as

$$\rho(x,t) \equiv |\psi(x,t)|^2 \sim |A(x,t)|^2.$$

A rather simple consequence (and yet crucial) can be derived from the fact that for systems where the number of particles does not change,

$$\rho_0(x_0,t_0)dx_0 = \rho(x,t)dx,$$
where \( \rho_0 \) is the initial density at some initial time \( t_0 \) and in one dimension both sides of the above equation represent number of particles. This immediately leads to the observation that,

\[
A(x, t) \sim A(x_0, t_0) \left( \frac{dx}{dx_0} \right)^{-1/2}
\]

which is a statement about the functional form of the amplitude at later times. Now comes the question - clearly, if the derivative indicated in the above equation vanishes, then the amplitude at some time \( t \) will become infinite! Is that physical? What does it mean? First of all let me point out that such singularities of the amplitude are not artifacts of our approximation and in fact one sees this in many everyday phenomena for e.g, focal point of rays in optics. These points at which the amplitudes diverge are known as caustics. To make some connection to what you might know at this point, caustics and turning points (for potentials) are one and the same for one dimensional time independent cases. In higher dimensions or more general equations all bets are off!

Notice that all of the statements we have made above still don’t mean we have interference since a single term cannot do so and one definitely needs more than one such complex exponentials to get some interference. This is not a problem since what we have written down as an asymptotic solution to the Schrodinger equation is not quite all correct and one does have many such terms. One of the reasons being that objects like classical actions are multivalued functions and we have to consider all possibilities and in fact a more general solution will be something like

\[
\psi(x, t) \sim \sum_b A_b(x, t) \exp \frac{i}{\hbar} S_b(x, t) + O(\hbar),
\]

where \( b \) denotes the various branches and pictorially one can get a feeling for this. Consider the following two dimensional phase space (one degree of freedom) sketch: In the above figure it is clear that if I pick some arbitrary
2.1. THE WKB APPROACH

$x_0$ then there can be quite a few branches for the momenta. To be fair we have to consider all these and later down we will show how important this is since all kinds of wonderfull things can be derived from this.

Now, up untill now we have been considering the time dependent case and what we will need more for this project is the time independent situation. It is rather easy to derive the equations in this case and I will just quote the results. At the zeroth order in $\hbar$ we have the classical Hamilton-Jacobi equation,

$$\frac{1}{2m} \left( \frac{\partial S}{\partial x} \right)^2 + V(x) = E,$$

which can be solved for one the one dimensional hamiltonians of the form $H(x, p) = p^2/2m + V(x)$ in a straightforward manner

$$S_b(x) = \int^x p_b(x', E)dx' \equiv \pm \int^x \sqrt{2m(E - V(x'))}dx',$$

where, as before, $b$ stands for the branch and there are only two in this situation.$^6$ At the next level by identifying $\rho = |A|^2$ one can write down

$$\frac{d}{dx}(\rho v) = 0,$$

where $v$ is the velocity. This immediately tells us that

$$A(x) = \frac{c_b}{|v_b(x)|^{1/2}},$$

where $c_b$ is a constant to be determined later. Putting all this together we have then the semiclassical approximation to the quantum energy eigenfunction as follows:

$$\psi_E(x) = \sum_b \frac{c_b}{|v_b(x)|^{1/2}} \exp \frac{i}{\hbar} \int^x p_b(x', E)dx'.$$

It is important to see that if the velocity vanishes (i.e., turning point which are caustics in this case only!) the wavefunction diverges! This is a “fly in the ointment” but something can be done about this and in a indirect way later on we will see that the buzzword is uniform solutions.

Of course we are not done yet - what about the $c_b$’s? It will turn out that they are just phases (but cannot be ignored) and the demonstration

$^6$It is important to note that the curve $H = E$ need not be a closed loop in phase space or even in one piece (tunneling) and the results hold. But classical trajectory on one of the disconnected pieces of $H = E$ will not go over to some other piece in real time.
of this will be longish. So for now I will stay away from it but just sketch the ideas which are due to the Russian V. P. Maslov and are indeed quite elegant. The idea is that if we could write semiclassical expressions for the wavefunction in position representation then we can equally well write one down in the momentum representation. This we would do as follows:

$$\phi_E(p) = \sum_b \frac{d_b}{|\tilde{p}(p)|^{1/2}} \exp \left( -i \frac{\bar{\hbar}}{\hbar} \int p x_b(p', E) dp' \right), \quad (2.29)$$

and notice the similarities to a fourier transform. The $d_b$'s are a different set of constants now. Now, here lies one of the important lessons in semiclassics - you see in quantum mechanics the two representations are exactly equivalent i.e., if you work with one or the other representation it does not matter and you should get the same observables and all that. In semiclassics the case is a bit different in that the two wavefunctions are not the exact fourier transforms but related by stationary phase fourier transforms. This is because we do not have exact wavefunctions but asymptotic ones and one has to be careful. In other words, if you have a semiclassical wavefunction in the position representation then you first write down the fourier transform of it and then evaluate the fourier integral by stationary phase methods. Now with this kind of semiclassical duality you demand consistency of results for things you know that should come out the same no matter what representation you are in and then you can relate the $c_b$'s and the $d_b$'s. Whew! that is making a long story short. So, the punchline is that in general we get

$$\psi_E(x) = \sum_b \frac{1}{|\hat{x}_b(x)|^{1/2}} \exp \left( i \frac{\bar{\hbar}}{\hbar} \left[ S_b(x, E) - \frac{\pi \hbar \mu_b}{2} \right] \right), \quad (2.30)$$

where the phase $\mu_b$ is known as the (you guessed it!) Maslov index.

This above was a rather quick introduction to WKB method and as to what it can do for you. Now, we are still left with the question we started this whole article with - what about tunneling? We still have to show how to get tunneling by using these ideas and in particular can we get tunneling amplitudes etc. by this technique as far as one dimensional case goes. In general given some one dimensional potential we can write down the form

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7The same kind of argument happens as far as working in energy and time representations go and this has given rise to quite a bit of activity in the recent years and some surprises!

8This index is what mathematicians would call as a topological invariant and gives rise to the 1/2 zero point energy for the harmonic oscillator! This whole aspect of the theory has some very beautiful (differential) geometry but it is not possible in this set of notes to get into that.
of the WKB wavefunctions in the classically allowed regions as long as we promise to stay away from turning points! In fact writing down semiclassical wavefunctions for classically allowed regions even in multidimensions is relatively straightforward as one can generalize the above arguments with little difficulty.

This would, in principle, let us find the quantized energy levels for our multidimensional system and the approximation gets better as we go to larger and larger quantum numbers (why?). The reason I am being careful is that in multidimensions there are quite a few subtleties that do creep in like resonances, destruction of tori to name a few, that one has to worry about. You see, as far as classical mechanics of conservative systems go, one dimensional systems are integrable and motion in phase space happens on 1-tori (for bound systems). In multidimensional (nonlinear) systems can have chaos developing due to nonintegrability and this means that not all of phase space has motion happening on nice smooth tori! As chaos sets in most of the tori are being destroyed!! So, if we do not have tori then what are we constructing our wavefunctions from and how do we get energy levels? Turns out, in the case of systems that are completely chaotic and thus have no tori left in phase space, one could rely upon the periodic orbits of the system (in phase space again!) to quantize. Let me end this little digression by pointing out that for the so called mixed systems for which phase space has both tori and stochasticity the problem of quantization is still an unsolved problem and we have not even gotten to the problem of describing tunneling for integrable systems yet in this set of notes! 

Ok, so in the classically allowed regions we can write down the WKB wavefunctions if we promise to stay away from caustics (multidimensions). We know why we are being so wary of turning points (or caustics, to be more general) - our primitive WKB wavefunctions blowup at such points (regions) and quantum mechanically this does not happen. Intuitively (and I am treading dangerous grounds here and implore you to take this with a grain of salt!) one expects that there would be a large probability of finding the particle at points where it is not moving! One mundane analogy is estimating the probability of finding a person in some city when he is moving around all the time as opposed to staying at his home (allright, this is a bad

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9By the way, tori is the plural for torus. The tori on which classical motion happens in phase space are known as Lagrangian manifolds and are central to quantize a system. In the formulas we have been writing down the index $b$ has to do with the branches of this manifold and certain consistencies that we demand from this lead to the Maslov index which in turn is quite important to get the quantization just right.

10This leads to the Gutzwiller theory and trace formulas which we do not deal with here but not all loose ends have been tied in this case either!
one!). Large probability is one thing, and quantum mechanics supports this to some extent, but infinite probability - that is too much. So, what went wrong with our semiclassical analysis? Actually not too much, if we adhere to Maslov’s viewpoints, since caustics arise due to the geometry of the lagrangian manifolds in phase space and we are tied down to one particular representation as far as our wavefunctions go. If you switch representations then everything is fine and in some sense there are no caustics in phase space. This is kind of “handwavy” and I do not want to digress again since then I would have to call this article as a gentle introduction to digressions! Think of a one dimensional bound system like the harmonic oscillator and it is easy to imagine a large probability of finding the particle near the turning point but at the same time beyond the turning point into the region which would be labeled as classically forbidden region (CFR) the probability of finding the particle would be rather small. That makes sense since the potential keeps on rising becoming kind of an infinite wall which prevents the particle from getting free and going off to infinity! This is precisely the reason that quantum mechanical wavefunctions for the harmonic oscillator are such that at very large distances (to the right or left of the equilibrium point) the probability is essentially zero for finding the particle. Very close to the turning point however there is an exponentially small probability that the particle can tunnel so that we can find it just into the CFR.

- Take the one dimensional harmonic oscillator ground state quantum wavefunction and calculate probabilities for finding it away from the turning point into the CFR as a function of the distance.

So, how do we explain this using our semiclassical analysis and in particular how do we deal with turning points (in one dimensions for now) in our problem. Let us resign ourselves to being tied down to the coordinate representation and try to see if we can “smooth away the infinity at the turning point” i.e., come up with a uniform WKB approximation. This means we would have to look very closely at the region around the turning point and analyze the behaviour of our semiclassical wavefunctions there. Hopefully, this way we can also get that right exponential fall of wavefunction in the CFR that would give us tunneling!

The idea in a way originated in a paper by Miller and Good and now goes
by the name of *comparision equations*. Allright, so all of the arguments I am
going to make now are completely one dimensional and generalizing all this is
an open problem. In particular I am not going to go into the formal derivation
of equations and other things but just outline what the idea is. Consider a
potential and some energy $E$ which we are interested in as sketched below:
In this figure the classically allowed region is to the left of the turning point

$x_0$ and the CFR is to the right of $x_0$. First of all note that in the classically
allowed region since $E > V(x)$ the square of the momentum is *real* that is
$p^2(x) > 0$. But in the CFR $E < V(x)$ and thus $p^2(x) < 0$ which means the
momentum is pure imaginary. Now in the classically allowed region I can
write my usual WKB solution as follows

$$\psi(x) = \frac{1}{|p(x)|^{1/2}} \left[ c_R e^{i\phi} + c_L e^{-i\phi} \right], \quad (2.31)$$

where I have set

$$\phi(x) = \frac{1}{\hbar} \int_{x_0}^x p(x) dx + \frac{\pi}{4} \equiv \frac{1}{\hbar} S(x,x_0) + \frac{\pi}{4}. \quad (2.32)$$

Now since there is a turning point (caustic) and this is our usual Hamiltonian
we have two branches for the momentum and hence the two terms in the
WKB wavefunction. The $\pi/4$ has to do with the relative phase between the
branches as we discussed earlier. That is what it turns out to be if you work
it out. So all this we know how to write down. Now we come to the CFR
and here the momentum becomes purely imaginary and this means we can
write the wavefunction as

$$\psi(x) = \frac{1}{|p(x)|^{1/2}} \left[ c_G e^{K(x)} + c_D e^{-K(x)} \right], \quad (2.33)$$
where I have defined
\[ K(x) = \frac{1}{\hbar} \int_{x_0}^{x} |p(x)| \, dx. \]  
\[ (2.34) \]
Notice carefully that we have not just “substituted” \( p(x) \rightarrow i |p(x)| \) to get the wavefunction in the CFR from the wavefunction in the classically allowed region! The coefficients are all different and moreover there is no \( \pi/4 \) phase. This is an important point. All I know is that in the CFR the momentum (as far as one dimension is concerned) becomes purely imaginary and so the WKB form of the wavefunction must have some growing and damped exponentials. It too, as you approach the turning point, has problems! What I am trying to say here is that to begin with we could have started doing asymptotics on the equation
\[ \psi'' - \frac{|p(x)|^2}{\hbar^2} \psi = 0, \]
which is nothing but the Schrödinger equation for \( E < V(x) \). Then we would have discovered that equation above. We cannot and should not in general try to continue our asymptotic solutions from real to imaginary or complex cases\(^{11}\).

Now we are armed with WKB wavefunctions in the two regions and the question very clearly arises as to what is the connection between the various coefficients \((c_R, c_L)\) on one side and the coefficients \((c_G, c_D)\) on the other side? The resolution to this is usually called as the connection formulae and let me just mention how this comes about. The basic idea is this: Near a turning point one can approximate the potential by a linear function and this allows us to turn the Schrödinger equation into an exactly solvable equation! When one solves for such an linear potential then the solutions we get are called as the Airy and Biry functions. They are denoted by \( \text{Ai}(x) \) and \( \text{Bi}(x) \) respectively. The wonderfull thing about this is that the Airy and Biry functions themselves have asymptotic expressions corresponding to the two regions of interest to us. Well then, life is simple since we can just compare the asymptotic form of the \( \text{Ai}(x) \), \( \text{Bi}(x) \) with the asymptotic solutions we have before and come up with a relation between the coefficients. The asymptotic forms for the Airy and Biry functions are as follows: In the classically allowed region we have
\[ \text{Ai}(z) = \frac{1}{(-\pi^2 z)^{1/4}} \cos \left( \frac{2}{3} (-z)^{3/2} - \frac{\pi}{4} \right) \]
\(^{11}\)This is a subtle feature of asymptotic theories and one has to be very aware of this since otherwise we will get nonsense. Again I cannot go into details at this point of time and for your interest mention that this comes under the heading of Stokes phenomena in case you feel the urge to follow it up.
2.1. THE WKB APPROACH

\[ \text{Bi}(z) = \frac{-1}{(-\pi^2 z)^{1/4}} \sin \left( \frac{2}{3}(-z)^{3/2} - \frac{\pi}{4} \right), \]  
\[ \text{(2.36)} \]

and in the CFR the following asymptotic results hold

\[ \text{Ai}(z) = \frac{1}{2(\pi z)^{1/4}} \exp \left( -\frac{2}{3}z^{3/2} \right) \]
\[ \text{Bi}(z) = \frac{1}{(\pi^2 z)^{1/4}} \exp \left( \frac{2}{3}z^{3/2} \right), \]  
\[ \text{(2.37)} \]

where the relation between the variable \( z \) and the action is

\[ z = -\left[ \frac{3}{2\hbar}S(x, x_0) \right]^{2/3}. \]  
\[ \text{(2.38)} \]

Note that the branches corresponding to the 2/3 power are chosen so that for classically allowed regions \( z < 0 \) and for CFR \( z > 0 \). Comparing we find that the relation between our WKB wavefunction coefficients is given by

\[ \left( \begin{array}{c} c_G \\ c_D \end{array} \right) = \left( \begin{array}{cc} i & -i \\ \frac{1}{2} & \frac{1}{2} \end{array} \right) \left( \begin{array}{c} c_R \\ c_L \end{array} \right). \]  
\[ \text{(2.39)} \]

This above equation tells us how to connect up across various regions of our potential surface (one dimensional) and one can use this to find observables like tunneling splittings in a double well potential and tunneling rates in unimolecular potentials.

- Show the above relation between the coefficients by doing the comparison between the Ai, Bi functions and the WKB solutions.

I should warn at this point that I have skipped over certain subtleties that come about at this point and which have, historically, been a source of considerable acrimony between early WKBers! But this brief overview should have given you enough of a flavor as to what is this WKB approximation all about and why it is so hard to generalize it to multidimensions! To get a deeper and proper understanding of semiclassical approximations would require me to practically write a book - clearly not feasible since I myself am not at that stage as of yet. This is a sketch of what I have learnt from my “Gurus” - Bill Miller and Robert Littlejohn while I was still an impressionable
young graduate student. Let us hope that they at some point will plan on writing something which will make this fascinating subject accessible to a wider audience.
Chapter 3

Semiclassical Propagators - some perspectives

Well, let us say that you do have a super-duper computer with which you can do any quantum calculation - structure and dynamics. Afterall, chip speeds are getting faster (with uncertainty principle being the theoretical limit) and gigabytes are getting cheaper. So suppose you use this monster machine to do tunneling calculations for some interesting molecule which perhaps is being experimentally studied by your friend as well. Now, your friend tells you that with a similar molecule, which happens to have just one weakly coupled mode missing as compared to the original one, the tunneling effects are a thousand times amplified! Immediately we run to the monster machine, feed in this new molecule and out come the results - indeed the tunneling effects are enhanced by a very large amount. What now? It is perplexing to you and the experimental friend that just one measly, weakly coupled mode is making such a large difference. How does one account for this? One can look at the thousands of eigenvectors and eigenvalues over and over again but that is not going to be of much help. The point is that interpretation of what you compute can be quite difficult in quantum mechanics. Admittedly, there are ingenious ways of looking at the quantum data and some people are blessed with this art but nothing can replace the copious amounts of insights provided by the underlying classical dynamics of the system. However, we do not want to miss out on any interference effects\footnote{It is possible to question this quantumness of interference. Basically, whenever you have a wave like theory/interpretation which is linear one will invariably have interference effects. For example, classical Maxwell theory of electromagnetic fields has the full glory of interferences. One can start from the classical Hamilton-Jacobi theory and build a wave theory from it \textit{a la} Huygens then interference effects are natural. The only subtle thing is explaining the origins of a constant symbolized $\hbar$ in nature.} and hence the right thing to look at
is the semiclassical regime. In a sense then the knowledge of the underlying classical dynamics forms a perfect backdrop in order to understand what the quantum theory is predicting. Notice, I am being careful in not picking one theory over another as more fundamental. This, at least in my views, is not a done thing.

This quantum-classical correspondence is a very interesting and challenging problem which is definitely not settled yet. Almost every so-called quantum object has a classical counterpart. The semiclassical bridge is a bit tenuous right now since quantum theory is based on a linear differential equation whereas classical theory is based on nonlinear differential equations. For example, people have recently shown that with a bit of “noise” classical objects look more like quantum objects! So, studying dynamics from this classical-quantum correspondence perspective can be very rewarding.

3.1 Propagators - Quantum and Semiclassical

The word *propagator* clearly implies something which will propagate something. In other words, whenever you want to propagate some object then you will have or will need a propagator. In a very general sense then, the concept of a propagator is neither classical or quantum! What I mean is that whatever theory you have you will have propagators which are the heart and soul of that theory\(^2\). Essentially, there are two concepts - that of propagators and generators. These two are intimately linked. In order to propagate or evolve your system along some variable (think coordinate) there is a generator that generates this motion along that variable. So, if one wants to propagate in space then the generator of this space evolution is momentum. If propagation in angular space (rotations) is required then the generator is the angular momentum. Hamiltonian is the generator of time translations. Perhaps now the idea of conjugate variables becomes a bit clearer! In a very abstract sense, if \((A, B)\) are a conjugate pair of objects (dynamical variables, operators, functions whatever..) each one of this pair can act as a generator of evolution of the system along the other object. In other words, \(A\) can be viewed as the generator of translations in \(B\) and vice versa. Thus \((x, p_x)\) form a conjugate pair since \(p_x\) is the generator which evolves the system along \(x\). I could go on and on about this very general and elegant subject and formulate

\(^2\)This is more general than one tends to think at first blush. For example in the theory of continuous groups or *Lie groups* one has the concept of a generator of the group. There are structures which propagate you in this group space. The connection of Lie groups to physical situations basically revolves around this generator/propagator structures.
3.1. PROPAGATORS - QUANTUM AND SEMICLASSICAL

everything without any reference to quantum or classical theory as such. But let me not do that since that would take us away to far and far better people then myself have written about these things. Let me specialize to quantum theory for now and then semiclassize the arguments.

In quantum mechanics one is always interested in questions like what is the time evolved state of a system given I started with some initial state. Suppose your initial state at time $t_0$ is denoted by the ket vector $|\alpha, t_0\rangle$. What we need is how do we evolve this initial state in time $t$. So, we need an evolution operator, or a propagator which will propagate $|\alpha, t_0\rangle$ in time and give us some state $|\alpha, t_0; t\rangle$ at a later time $t$. Notice that the new state at time $t$ can be anything and $\alpha$ is just a convenient, compressed index which could actually be a string of indices (quantum numbers) which are required to characterize a state. Ok, from the ramblings in the previous paragraph you know that it is the Hamiltonian operator $H$ which is the generator of time translations and thus the propagator must be related to $H$. But what is this relation? If you have not seen this before...here it is... This is not entirely rigorous, but I think the message will be heard. First up let us say that our time evolution operator or time propagator $U(t, t_0)$ must propagate i.e.,

$$|\alpha, t_0; t\rangle = U(t, t_0)|\alpha, t_0\rangle. \quad (3.1)$$

Now, what are reasonable things to expect from this $U$? Well, it is definitely reasonable to say that we can first evolve from $t_0$ to $t_1$ and then from $t_1$ to $t$ and we should end up with the system at time $t$. In other words,

$$|\alpha, t_0\rangle \rightarrow |\alpha, t_0; t_1\rangle \rightarrow |\alpha, t_0; t\rangle, \quad (3.2)$$

which is algebraically written as $U(t, t_1)U(t_1, t_0)|\alpha, t_0\rangle = |\alpha, t_0; t\rangle$. This is some kind of a composition law for this time propagator. This is an important property since it allows us to build up a long time evolution by smaller time evolutions! Thus, $U(t, t_1)U(t_1, t_0) = U(t, t_0)$. Secondly, say the initial state is normalized i.e., $\langle \alpha, t_0 | \alpha, t_0 \rangle = 1$. Then the final state at time $t$ must also be normalized i.e., $\langle \alpha, t_0; t | \alpha, t_0; t \rangle = 1$. More generally we are demanding that the length of our vector must not change under this time evolution. This is again reasonable since we want $U$ to be a linear operator. In other words for two states $|\alpha\rangle$ and $|\beta\rangle$

$$U(c_\alpha|\alpha\rangle + c_\beta|\beta\rangle) = c_\alpha U|\alpha\rangle + c_\beta U|\beta\rangle. \quad (3.3)$$

In a way this can be anticipated since we want to retain the usefull notion of superposition and the resulting interferences in quantum theory. If $U$ were not a linear operator then we would have possibly an entirely different
theory whose equations of motion are nonlinear! Thus demanding $U$ to be a linear operator implies time evolution is a linear transformation and linear transformations do not change lengths\(^3\). Thus it all boils down to saying that if the initial state is normalized to unity then the states at all later times must also be normalized to unity. This implies then the unitary property of the time propagator

$$U^\dagger U = U U^\dagger = 1.$$  \hfill (3.4)

As an aside, this whole demand on $U$ being unitary and, as you will see later, hence the Hamiltonian being hermitian is questionable. I mean, at this stage we want things this way so that observables are real numbers. I do not see yet why we are so stubbornly tied down to real observables etc. in the middle of this morass of complex objects. It seems like demanding the unitarity of $U$ is subjecting the theory to our prejudices!

Suppose now we are interested in very small time propagation \(i.e.,\) from the state at time $t_0$ to the state at a later time $t_0 + dt$. This will be achieved by the infinitesimal propagator $U(t_0 + dt, t_0)$ which should obviously satisfy

$$\lim_{dt \to 0} U(t_0 + dt, t_0) = 1,$$  \hfill (3.5)

and we expect for very small $dt$ the difference should be also linear in $dt$. Well, all this is begging for a Taylor series approach at this point and one can write

$$U(t_0 + dt, t_0) \approx 1 + \mathcal{C} \, dt,$$  \hfill (3.6)

where $\mathcal{C}$ is some operator with dimensions of inverse time that we have to determine. Well, using the unitarity property we immediately see that to order $dt$

$$\mathcal{C}^\dagger = -\mathcal{C},$$  \hfill (3.7)

which implies that $\mathcal{C}$ is a purely imaginary object. So let us pick $\mathcal{C} = -i \Omega$ and clearly this implies $\Omega$ is hermitian \(i.e.,\) $\Omega^\dagger = \Omega$. The minus sign is essentially to conform to the standard conventions. Putting all this together our infinitesimal time propagator becomes

$$U(t_0 + dt, t_0) \approx 1 - i \Omega \, dt.$$  \hfill (3.8)

Now, clearly $\Omega$ as an operator has the dimensions of inverse time or frequency

\(^3\)Think of linear algebra in a plane for example. Linear transformations like translation, rotation etc. will not change the length of a vector. Also note that for a complex valued object $a$, it is the modulus squared $a^*a$ which is the length and invariant under linear transformations.
3.1. PROPAGATORS - QUANTUM AND SEMICLASSICAL

which is naturally identified\(^4\) with \(H/\hbar\). Now, we can use the compositional property of \(U\) (you must be wondering when that was going to be used!)

\[
U(t + dt, t_0) = U(t + dt, t)U(t, t_0) = \left(1 - \frac{iH dt}{\hbar}\right)U(t, t_0), (3.9)
\]

where \(t - t_0\) need not be small at all. Hence we get

\[
U(t + dt, t_0) - U(t, t_0) = -\frac{iH}{\hbar} dtU(t, t_0), (3.11)
\]

and this immediately leads to the Schrödinger equation for the time propagator

\[
i\hbar \frac{\partial}{\partial t} U(t, t_0) = HU(t, t_0). (3.12)
\]

Of course the above equation immediately implies the time dependent Schrödinger equation for the state kets (show this). We still have to get the finite time form for the time propagator itself. To do this, divide the time interval \(t - t_0\) into \(N\) smaller ones and then put them all together by using the infinitesmall versions. Now, let \(N \to \infty\) and thus we get the required time propagator as

\[
\lim_{N \to \infty} \left[1 - \frac{iH \tau}{\hbar}\right]^N = e^{-iH(t-t_0)/\hbar}, (3.13)
\]

where we have used the notation \(N \tau = t - t_0\). For Hamiltonians with explicit time dependence the results can be generalized\(^5\) but for us this result is more than enough. Usually when people say propagator they mean this time propagator although the notions are very general.

Allright, now that we have the time propagator in hand we possess a very powerful tool. Using this one can calculate any transition amplitude one requires! The probability for such a transition is of course proportional to the modulus square of the amplitude. So, for any process you can think of this will come in handy. Well, Feynman definitely thought so and developed

\(^4\)Of course one can raise a hue and cry about this \(\hbar\) business. This can be cleaned up to some extent by just working with the \(\Omega\) all thorough and then writing the equation of motion for any operator in the Heisenberg representation. If then one compares with the classical Liouville equation of motion, it becomes apparent that \(\Omega\) must be proportional to \(H\) with the proportionality constant dimensionally having inverse \(\hbar\) dimensions. But this is a digression that I do not want now!

\(^5\)For example, if indeed \(H = H(t)\) but the \(H\) at different times commute then \(U(t, t_0) = \exp\left(-\frac{i}{\hbar} \int_{t_0}^{t} dt'H(t')\right)\). If the different time commutator does not vanish then one has to be more careful and it leads to the so called Dyson series.
the whole path integral approach to quantum theory via this time propagator. Feynman was led to this by a remark by Dirac and you can read this up in §. The propagator itself is an operator and as usual depending on the various contexts we would require the matrix elements of the propagator in various representations. For example, say we want the correlation function \[ \langle \phi | \psi(t) \rangle. \]

The absolute squared of this correlation function when \( \phi \equiv \psi \) is the survival probability. To calculate this using the propagator we would do the following:

\[
\langle \phi | \psi(t) \rangle = \langle \phi | e^{-iHt/\hbar} | \psi \rangle \\
= \int_{\mathbf{q}_1, \mathbf{q}_2} \phi^*(\mathbf{q}_1) \langle \mathbf{q}_1 | e^{-iHt/\hbar} | \mathbf{q}_2 \rangle \psi(\mathbf{q}_2) \\
= \int_{\mathbf{q}, \mathbf{p}} \phi^*(\mathbf{q}) \langle \mathbf{q} | e^{-iHt/\hbar} | \mathbf{p} \rangle \psi(\mathbf{p}) \\
= \int_{\mathbf{p}_1, \mathbf{p}_2} \phi^*(\mathbf{p}_1) \langle \mathbf{p}_1 | e^{-iHt/\hbar} | \mathbf{p}_2 \rangle \psi(\mathbf{p}_2) \\
= \sum_{\mathbf{m}, \mathbf{n}} \langle \phi | \mathbf{m} \rangle \langle \mathbf{m} | e^{-iHt/\hbar} | \mathbf{n} \rangle \langle \mathbf{n} | \psi \rangle.
\]

In the above we have done the standard trick of inserting unity of various kinds. The initial state that we started out with does not have to be an energy eigenstate and in the last avatar of this formulae we have inserted a complete set of energy eigenstates (assumed to be discrete). One thing clear from this is that depending on the symmetry, convenience, likes and dislikes, you can work in a particular representation and then you will need the propagator matrix elements in that representation. Notice that I have also used a “mixed” representation of \((\mathbf{p}, \mathbf{q})\). There is nothing strange about this and in some instances can be very useful. Now, all of the above expressions are related to one another through some transformation or other. This is to be expected since whatever observables we are calculating are insensitive to the representation - nature does not care about what coordinate system we use! For example you know very well that in quantum theory the coordinate space wavefunction \( \psi_\alpha(\mathbf{q}) \equiv \langle \mathbf{q} | \alpha \rangle \) and the momentum space wavefunction of the same state \( \phi_\alpha(\mathbf{p}) \equiv \langle \mathbf{p} | \alpha \rangle \) are fourier transforms of each other

\[
\phi_\alpha(\mathbf{p}) = (-2\pi\hbar)^{-d/2} \int_{\mathbf{q}'} \exp \left( -\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{q}' \right) \psi_\alpha(\mathbf{q}') .
\]

The \( d \) here refers to the dimensionality of the system. Note that if we pick \( |\alpha\rangle = |\mathbf{p}'\rangle \) then this implies that (show this):

\[
\langle \mathbf{q} | \mathbf{p} \rangle = (2\pi\hbar)^{-d/2} \exp \left( \frac{i}{\hbar} \mathbf{p} \cdot \mathbf{q} \right) \\
\langle \mathbf{p} | \mathbf{q} \rangle = (-2\pi\hbar)^{-d/2} \exp \left( -\frac{i}{\hbar} \mathbf{q} \cdot \mathbf{p} \right).
\]

30
As emphasized by Dirac the above two equations are equivalent to the fundamental commutation relations $[q_i, p_j] = i\hbar\delta_{ij}$. Can you demonstrate this? All this is very beautiful and in fact the above transformations hold as long as the variables involved are canonically conjugate\(^6\).

It is clear from the above arguments that whatever transition amplitude you need for some process, one is interested in the matrix elements of the time propagator. Fine, so now we ask the crore rupee question - How do you get or compute the matrix element $\langle q_2 | \exp \left(-\frac{i}{\hbar}Ht \right) | q_1 \rangle \equiv K(q_2, q_1; t)$? All along in this set of notes I have been calling something as an propagator whereas usually it is the $K$ that people call propagator. As you can see it does not matter very much but the reason for this is that if one wants to transport some wavefunction at initial time $t_0 = 0$ to time $t$ then this can be done as follows:

$$\psi(q_2, t) = \int_{q_1} K(q_2, q_1, t) \psi(q_1, 0). \quad (3.17)$$

Anyways, with this in mind, we come back to the crore rupee question. First of all note that I can think of $K(q_2, q_1, t)$ as a transition amplitude or probability amplitude for a particle to go from the space-time point $(q_1, 0)$ to the space-time point $(q_2, t)$. Now note how close this point of view is to the trajectories in classical theory! The transition amplitude is governed by the Hamiltonian...good, because that is what it is in classical mechanics too..remember, Hamilton’s equations of motion. However, now the question arises - how does the evolution happen? I mean what “trajectory” is this particle taking for the evolution in space-time $(q_1, 0) \rightarrow (q_2, t)$?

For the time being let us visit classical land and ask the very same question \textit{i.e.}, how does one find the motion of a particle from $(q_1, 0) \rightarrow (q_2, t)$? Notice here something which is (or will be) amusing as well as important. I could have asked the question in a different way - how does the evolution $(q_1, p_1, 0) \rightarrow (q_2, p_2, t)$ happen? Here, I am starting at time zero with some initial position and momentum and asking for a classical trajectory which at time $t$ gives my particle some other position and momentum. Clearly there can be only one answer. This follows from the fact that in phase space classical trajectories do not cross\(^7\). So, the message is that if I fix a initial point in phase space then solution to the Hamilton’s equations of motion

\(^6\)We could go off on a tangent here and show all the elegant results. You see, unitary transformations in quantum theory correspond to the canonical transformations in classical theory. One could develop a whole new thing which is not tied down to any representation whatsoever.

\(^7\)This better be the case since otherwise the solutions of our classical evolution equations will be nonunique!
gives me a unique trajectory and hence in a time \( t \) a unique point in phase space. Now, the question we started out with is a bit different. We are not starting with some initial point in phase space but we are asking if I start my system out at \( t = 0 \) at some initial position \( q_1 \) and demand that the final position at a later time \( t \) is \( q_2 \) then what are the possibilities? The difference between the two kinds of questions has to do with different ways of solving the classical equations of motions which are of course differential equations. In one case it is the solution from an initial value perspective whereas in the case we are interested in it is from the boundary value perspective. The interesting thing about the boundary value viewpoint is that there can be more than one classical trajectory that can take you from \( q_1 \) to \( q_2 \) in a time interval \( t \). Well, this is not a surprise since I am only interested in getting from here to there in some fixed time \( t \) and I can choose any momentum to do this job! Think about a harmonic oscillator and it will become clear. By the way do convince yourself, by an actual calculation, that there are an infinite (yes, infinite) number of classical trajectories for a particle behaving harmonically to go from one position to another in some time \( t \). It is obvious that for such more then one trajectory solutions, classically, one needs a bound system. Now in the initial value case you would just solve for the Newton or Hamilton equations of motion subject to the initial conditions. The Hamilton equations of motion are

\[
\dot{q} = \nabla_p H(q, p) \\
\dot{p} = -\nabla_q H(q, p).
\]

(3.18)

What about the boundary value case? Well, this is the so called Lagrangian approach to classical mechanics. You see, in the Hamiltonian mechanics the whole story unfolds in phase space whereas as far as Lagrangian mechanics is concerned it all happens in the configuration space. Now, let me derive for you something that you already know..but a bit more carefully than what you might have seen. Imagine the following space of paths:

\[ \mathcal{S} = \{ \text{All conceivable } q(t) \text{ such that } q(t_1) = q_1 \text{ and } q(t_2) = q_2 \}^8. \]

---

\(^8\)The space \( \mathcal{S} \) is actually parameterized by \((q_1, t_1, q_2, t_2)\) but we will not explicitly indicate it.
Now consider the Action functional

\[ A[q(t)] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t), t) dt, \quad (3.19) \]

where \( L \) is the Lagrangian and \( q(t) \in \mathcal{S} \). Why are we defining this functional? Right now, I am saying that you have two spacetime points and one is imagining all possible paths connecting the two points. The question here is that, is nature completely indiscriminate at this level? Is or are there preferred paths? This is a very delicate question. We are trying to guess from our observations. You throw a stone from here to there and every time (within your observational resolution) it seems to take a very particular path from here to there. The stone is thrown many times, by many people and at many places...same conclusion! So, does that prove that nature is discriminate? No...it only strengthen the belief that perhaps nature discriminates...it could have chosen all these wonderful paths but only one (or a few) is liked by nature. This, I hope you appreciate, is a rather deep mystery of nature. I could very well give you a very historic flavor to this whole business but will restrain myself. The burning question in people’s mind was this - how would the physics pick out the path(s) that nature seems to prefer? I mean, afterall the \( \mathcal{S} \) space is infinite dimensional so is there a reason that some paths are “special”? Ok, so let me get right to the point...to make a long story short.. Hamilton, Fermat, Maupertius and many others realized that the paths that nature picked are the ones such that the action functional is stationary with variations in the path. Mathematically, a path \( q(t) \in \mathcal{S} \) is physically realizable iff

\[ \frac{\delta A}{\delta q(t)} = 0. \quad (3.20) \]

This is known as Hamilton’s principle. As you know, this directly leads to the Euler-Lagrange equations\(^\text{10}\) of motion since

\[ \frac{\delta A}{\delta q(t)} = \frac{\partial L}{\partial q} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}} \right). \quad (3.21) \]

Now, the important thing to realize here is that Hamilton’s principle says how to pick such supposedly special paths out of the \( \mathcal{S} \) space. But nothing is said about second variation in \( A \)! In general the \( \delta^2 A \) do not vanish\(^\text{11}\). Note also

---

\(^9\) Functionals are generalization of functions. See Ami’s notes hereafter referred to by \(^\flat\).

\(^{10}\) The variation represented by \( \delta \) is really a functional differentiation.

\(^{11}\) The second variation of \( A \) has its own interesting features. It should be clear that the usage “principle of least action” is wrong and it should be called principle of stationary
that nothing says that the solution has to be unique, or even that it should exist. The solution could be in complex $t$, or there could be $1, 2, \ldots \infty$ of solutions.

Ok, with that interlude, back to the question at hand - what "trajectory" does nature pick at a quantum level? Feynman's answer, with inspiration from Dirac (see §), is that nature does not discriminate anymore!\footnote{This is an appropriate place to go back, historically, and reexamine what led people to postulate the stationary action principle in classical mechanics. Maybe, nature is democratic even classically and we are missing something. Perhaps, we needed the microworld to realize that nature is indeed democratic!}

Can one "rationalize" Feynman's argument? I am not going to attempt it in any detail here. You should read the Dirac Sowjetunion paper and then the Feynman Reviews of modern physics paper. In addition, it is important to have your own views about this. The visit to the classical land has definitely taught us something crucial - in this boundary value kind of question we need to think about the Lagrangian first. So, somehow to calculate the $K(q_2, q_1, t)$, we would at some stage or the other have to invoke the Lagrangian. Although both Lagrangian and Hamiltonian perspectives are equivalent, the Lagrangian approach is more fundamental. For conservative systems the Hamiltonian approach is more natural, but if the total energy is not conserved then we are better off dealing with the Lagrangian. So, what was this Dirac insight which led to Feynman’s path integrals? One way of looking at it is in §. Here, let me borrow from Dirac's own exposition but done in a slightly modern notation. Now, what Dirac has written is absolutely clear and it would be sacrilegious on my part to claim any originality here! I am just following the master. In particular you will notice the carefulness of Dirac’s approach and as to how damn close we are to the classical world.

First, consider classical mechanics and give a definition of canonical transformations. I will use a one dimensional notation and it is easy to generalize to as many degrees of freedom as you like. Suppose we have two sets of independent variables $(p, q)$ and $(P, Q)$. Consider a transformation from one set to another i.e., $(p, q) \to (P, Q)$. If this transformation is canonical then the Jacobian of the transformation is equal to one.

$$
\left| \frac{\partial (P, Q)}{\partial (p, q)} \right| = 1.
$$

In addition, if the transformation is canonical then the form of the equations of motion changes. In fact one can ask the question as to is it possible that the action is indeed minimum for some cases or whether it is a minimum for certain time etc. For all this one has to study $\delta^2 A$ in more detail and has interesting connections to Morse theory and some rich topology. If you are really interested, you should get started by reading Schulman's book on path integrals.
of motion remains the same \( i.e., \) in the new \((P, Q)\) system the equations of motion are again \( \dot{Q} = \partial_P H(P, Q) \) and \( \dot{P} = -\partial_Q H(P, Q) \). Now, in general any two variables from the above four can be chosen as the independent variables to describe the system. This could be \((p, Q), (P, q), (q, Q), (p, P)\). Note that I have taken one new and one old variable. This is because if one wants to construct a canonical transformation one would need something that generates the transformation\(^{13}\). The variables \((p, q)\) or \((P, Q)\) are already canonically conjugate pairs. Suppose we choose one of the above “mixed” representations, say \((q, Q)\). This would imply that the other variables must be functions of \((q, Q)\). Thus, \( p = p(q, Q) \) and \( P = P(q, Q) \). It is also obvious that \( H(p(q, Q), q) = H(P(q, Q), Q) \). This implies that, by differentiating with respect to \( q \) holding \( Q \) fixed, \[
\left( \frac{\partial H}{\partial p} \right)_q \left( \frac{\partial p}{\partial q} \right)_Q + \left( \frac{\partial H}{\partial q} \right)_p \left( \frac{\partial P}{\partial q} \right)_Q = \left( \frac{\partial H}{\partial P} \right)_Q \left( \frac{\partial P}{\partial q} \right)_Q .
\] (3.23)

Note that the derivatives have to be done properly and with the understanding that now \((q, Q)\) are the independent variables. Now, if these are canonically related variables then, we get \[
\dot{q} \left( \frac{\partial p}{\partial q} \right)_Q - \dot{p} = \dot{Q} \left( \frac{\partial P}{\partial q} \right)_Q ,
\] (3.24)
and observing that \( \dot{p} \equiv \frac{dp}{dt} \) we have \[
- \left( \frac{\partial p}{\partial Q} \right)_q = \left( \frac{\partial P}{\partial q} \right)_Q .
\] (3.25)

Show that the above is correct. Clearly, if we have a function \( F(q, Q) \) such that \( p(q, Q) = \partial_q F(q, Q) \) and \( P(q, Q) = -\partial_Q F(q, Q) \) then everything works. This function \( F(q, Q) \) is known as the generator of the canonical transformation \((p, q) \rightarrow (P, Q)\). Since there were four possible mixed representations we could have started with, there are thus four such generating functions. All four of the generating functions are related by Legendre transforms. In reality, these are implicit equations that have to be solved in order to construct the transformation itself. For example, first use the equation \( p(q, Q) = \partial_q F(q, Q) \) to solve for \( Q(q, p) \) and substitute this expression for \( Q \) into the other equation \( P(q, Q) = -\partial_Q F(q, Q) \) to get \( P(q, p) \equiv P(q, Q(q, p)) \). In general we can have many solutions and multivaluedness is the rule rather than the exception. In practice though, the “disentangling” of the generator relations to get

\(^{13}\)The word generator here is not something different from what we have been talking about all along. This is not an accident either!
the explicit form for the new variables in terms of the old variables can be rather difficult. I will not say anything more about this topic. Suffice it to say that $F(q, Q)$ is the generator which generates the canonical transformation. Of course, nothing pious about $F$ as it could equally well be $G(q, P)$. Ok, so now let us go to quantum land and see what happens. Just like in classical case, pick two representations - one in which $\hat{q}$ is diagonal and another in which $\hat{Q}$ is diagonal. Continuing the analogy, there will be a “transformation function” which connects the two representations. The question is that what is this transformation function. You see, in classical land it was the function $F(q, Q)$. To do this first notice the following identities

$$\langle q | \hat{A} | Q \rangle = \int_{q'} \langle q | \hat{A} | q' \rangle \langle q' | Q \rangle,$$

(3.26)

for any operator $\hat{A}$. From this it follows that (show this!):

$$\langle q | \hat{q} | Q \rangle = q \langle q | Q \rangle,$$

(3.27)

$$\langle q | \hat{p} | Q \rangle = -i\hbar \partial_q \langle q | Q \rangle,$$

and

$$\langle q | \hat{Q} | Q \rangle = Q \langle q | Q \rangle,$$

$$\langle q | \hat{P} | Q \rangle = +i\hbar \partial_Q \langle q | Q \rangle.$$

(3.28)

Now, just as in the classical case, we are thinking of $\hat{p} = \hat{p}(\hat{q}, \hat{Q})$ and similarly for $\hat{P}$. This of course means that

$$\langle q | \hat{p}(\hat{q}, \hat{Q}) | Q \rangle = p(q, Q) \langle q | Q \rangle,$$

(3.29)

which, as Dirac points out, is remarkable since it provides us with a connection between $\hat{p}(\hat{q}, \hat{Q})$ which is a function of operators and $p(q, Q)$ which is a function of numerical variables. Now, denote $\langle q | Q \rangle \equiv e^{iB(q, Q)}$ which is fine since any complex object can be written this way. This implies that

$$\langle q | \hat{p} | Q \rangle = p(q, Q) \langle q | Q \rangle = \hbar \partial_q B(q, Q) \langle q | Q \rangle,$$

(3.30)

Thus we get the following, miraculous, equation

$$p(q, Q) = \hbar \partial_q B(q, Q).$$

(3.31)

\[^{14}\text{Here, there is a subtlety. You have to have things well-ordered in } (\hat{q}, \hat{Q}). \text{ Ordering is crucial since these are operators which might not necessarily commute. Afterall, } Q = Q(q, p). \]
Similarly, we get the other part of the pair of equations as

\[ P(q, Q) = -\hbar \partial_Q B(q, Q). \tag{3.32} \]

If you compare this to the classical counterparts it is easy to see that \( \hbar B(q, Q) \leftrightarrow F(q, Q) \). Thus the generator of the transformation in quantum land and the classical land are the same modulo \( \hbar \). Thus, \( \langle q | Q \rangle = e^{iF(q,Q)}/\hbar \).

Now, we are ready for the generalization. In classical mechanics, the dynamical variables \((q, p)\) at a time \( t = 0 \) are connected to the dynamical variables \((q(t), p(t))\) at a later time \( t \) through a generating function (known as the action) which is nothing but the time integral of the Lagrangian. This should hold in quantum mechanics as well and thus the transformation function \( \langle q(t) | q(0) \rangle \) must correspond to \( e^{iS/\hbar} \). This, in a nutshell, is Dirac’s observation. Feynman took this up and made the meaning of the “corresponds to” phrase sharper which led to the path integral theory of quantum mechanics.

So now let us come back to the crore rupee question (a crore rupees is a lot of money and that is why we keep coming back to it!). The probability amplitude we are looking for is \( \langle q_2, t | q_1, 0 \rangle \). I am using one dimensional notation to simplify writing things down and will indicate the multidimensional case at the end. For now we are in the Schrödinger representation. In reality, it is the Heisenberg representation that is closer to classical mechanics. Recall that in the Schrödinger case the state kets move with time whereas they are stationary in the Heisenberg case. These are just different representations and hence finally all things observable must come out the same. In the Heisenberg picture what we are looking for is written as \( \langle q_2, t | q_1, 0 \rangle \). Thus, this makes direct contact with the Dirac idea. We still interpret \( \langle q_2, t | q_1, 0 \rangle \) as the probability amplitude for a particle prepared at \( t = 0 \) with position eigenvalue \( q_1 \) to be found at a later time \( t \) at the position \( q_2 \). So, in order to compute this object we have to calculate the action associated with it. Now computing an action also requires the specification of a path! Allowing for nature to be democratic we say that all possible paths have to be taken into account. Let me not derive the path integral for you but just quote the result\(^{15}\)

\[ \langle q_2, t | q_1, 0 \rangle = \int_{q_1}^{q_2} \mathcal{D}[q(t)] \exp \left[ \frac{i}{\hbar} \int_0^t dt L(q, \dot{q}) \right], \tag{3.33} \]

\(^{15}\)This is not very difficult to derive and you can look into any good quantum mechanics book. Basically, you subdivide the total time \( t \) into smaller times by writing \( e^{-iHt/\hbar} = (e^{-iH/\hbar N})^N \) and insert a resolution of unity (complete set of states) between each exponential factor. Thus effectively one imagines computing the propagator for smaller times \( \Delta t \equiv t/N \) since for very small times useful approximations can be made to the propagator. The prefactor is something that you will have to be careful with.
where the $\int_{q_1}^{q_2} D[q(t)]$ is an infinite dimensional integral operator

$$\int_{q_1}^{q_2} D[q(t)] \equiv \lim_{N \to \infty} \left( \frac{m}{2 \pi \hbar \Delta t} \right)^{(N-1)/2} \int_{q(N-1)} q_{(N-2)} \cdots \int_{q(2)} \int_{q(1)}$$

(3.34)

So, this was Feynman’s contribution as inspired by Dirac’s remark. The important thing here is that all conceivable paths are contributing as opposed to the classical stationary path(s) alone. By the way, one can wonder if it is possible to have a path integral approach from a phase space perspective. We have been doing what is known as the configuration space approach. It is kind of possible but there are difficulties and let me not digress into that for now. From a physical point of view (if one can call it that!) the fact that all paths are important is not too strange. The uncertainty principle says that you cannot specify both position and momentum to arbitrary precision. So, for each precisely specified space-time point along a classical trajectory the uncertainty in the conjugate momentum is large which naively means large uncertainty in velocity at a given position. Thus almost any position from a given specified initial position is possible and hence taken into account in the path integral. So, there you have it...if you can do the path integral then you can get the propagator and then anything else you need.

### 3.2 Semiclassifying things

The path integral approach outlined in the previous section is quite powerful but also difficult. You should try to solve for the case of a one dimensional harmonic oscillator. Perhaps one does not need all of those infinite paths. What if we retained only the classical paths? What if we retained classical plus “some” paths? The Feynman prescription attaches a phase and an amplitude with each chosen path contributing to the transition probability. It is the phase factor which makes things interesting. I mean all these interference effects and all that would not be there if it were not for the phase factors. This phase factor is the ratio of the action for a particular path to the Planck constant $\hbar$. It is wonderful that nature has arranged things in such a delicate fashion. You see, for many many years before the advent of the “quantum revolution” people like Hamilton, Jacobi, Lagrange, Poisson, Euler, Poincaré knew that phase space was a very natural setting for classical dynamics. The fact that $pq$ has the dimensionality of $\hbar$ (perhaps I should say it the other way around) is quite a miracle by itself. I cannot go too much into things to illustrate the nice properties of the action at this juncture\textsuperscript{16} Let me just

\textsuperscript{16}You must read Arnol’d for details. For example the so called Poincaré-Cartan form $dS = p \, dq - H \, dt$ plays a very fundamental role in classical dynamics and has some very
say that this happy coincidence(?), possibly, has very significant geometric meaning. Not all of it is understood as of yet.

Let us come back to the phase factor. Clearly, it is dimensionless. Now, notice that in the limit that the ratio goes to infinity we encounter an essential singularity. Basically what this means is that the complex exponential will oscillate violently. As a result the sum over paths for the propagator \( \langle q_2, t | q_1, 0 \rangle \sim \sum_{\text{paths}} e^{iS/\hbar} \) will essentially be zero. What does this mean? Well, take a very simple example. Suppose you take the function \( f_n(x; \delta x) \equiv \cos(n(x + \delta x)) \pm \cos(n(x - \delta x)) \). Now consider \( \int_0^{2\pi} f_n(x; \delta x) dx \).

In the limit \( n \to \infty \) you will see that the integral vanishes! Of course what we have is a more general situation like \( \cos(n g(x)) \) but the arguments are very similar. You just have to work a little harder to show things. Continuing along the same lines you should prove to yourself that a function like \( \cos(nx) \) will have about \( 2n \) zeroes in the range \( x \in (0, 2\pi) \). This means, as \( n \) gets larger and larger the function oscillates more and more within a fixed range. This is what one is talking about when the limit \( S/\hbar \) being large is being considered. Things just oscillate too much over too short a range and the net effect is nothing. The whole Young’s double slit experiment situation for electrons versus cricket balls should come into “focus” at this stage. Anyways, if this were the end of the story then all this delicate balancing act of nature etcetera I talked about will be for nothing! For now, notice that if I consider a function of the form \( f = e^{iS_1/\hbar} + e^{iS_2/\hbar} \) then \( |f|^2 \sim \cos^2((S_1 - S_2)/2\hbar) \). Thus if \( S_1 - S_2 >> \hbar \) then it is again going to oscillate like crazy and there will be no substantial contribution to its integral. Coming back to our elementary example, if I now think of terms of the form \( \cos(nf(x)) \) for some general function \( f(x) \) then things get interesting. As one takes the \( n \to \infty \) limit the integrals do not vanish in general! You see, the integrand itself is almost zero everywhere but values of \( x = \bar{x} \) such that \( f'(\bar{x}) = 0 \). You should try to show this to yourself\(^{17}\). Thus, if the function \( f(x) \) has stationary points then there could be\(^{18}\) nontrivial contributions. This, in a sense, is the starting elegant geometric structures associated with it. All this can be learnt/taught if one knows sufficient differential geometry and topology. It is amusing to quote Arnol’d from his book - “Hamiltonian mechanics cannot be understood without differential forms”. For a mathematically advanced, terse introduction to semiclassics refer to Arnol’d appendix 11.

\(^{17}\)You have to do some expansions here. In analogy, consider a function \( g_n(x; \delta x) \equiv \cos(nf(x + \delta x)) \pm \cos(nf(x - \delta x)) \) and start by expanding \( f(x \pm \delta x) \). Then expand \( f(x) \) itself around some \( \bar{x} \) and do the grind (consistently). Finally, you will end up with integrands of the kind \( \cos(nf'(\bar{x})(x - \bar{x})) \) which clearly will remain finite in the limit \( n \to \infty \) if \( f'(\bar{x}) \) vanishes. This is handwavy stuff but convinces you that things atleast get interesting.

\(^{18}\)I am being careful here. The various contributions from the stationary points of the function could conspire to give nothing!
point for semiclassics. The same line of reasoning leads us to believe that dominant contribution to the path integral will come, in the limit that actions are much larger than $\hbar$, from trajectories such that $\delta S = 0$. Well, that condition is nothing but Hamilton’s principle and so the main contribution, in this limit, is from the classical trajectories. This is very pretty and very much an example of a miracle! Thus, in the path integral sum, the various phases differ very much and tend to cancel each other when typical actions involved are much larger than $\hbar$. The exception to this happens in “regions” around the classical paths where the phases do not vary much to first order and thus constructive interference can happen. However, when typical actions are comparable to $\hbar$ then the integrals are in general nonzero whether or not there are classical paths around. Put another way, in the classical limit, the major contribution comes from classical paths and paths “nearby”. Otherwise the classical paths, as implied by Hamilton’s principle, do not have to be the main players. All this can be made quite rigorous using the formulation of stationary phase method for evaluation of integrals of the type $\int e^{if(z)}$ where in general $z$ is complex. This sort of semiclassical technique is used widely in many areas of science and engineering (not always properly, of course!). For example, in field theories, the so called “one-loop” corrections are nothing but a stationary phase or $O(h)$ result. Analogies to optics i.e., geometric optics vs wave optics in some sense was a precedent to all this. The mathematical basis/theory for these go under various names - geometric quantization, pseudo-differential operators, microlocal analysis and what not.

Anyways, now let us turn our attention to the propagator itself. Based on what I have rambled about in the previous paragraphs, it is clear that one could write something like this in the classical limit:

$$
\langle q_2, t|q_1, 0 \rangle_{sc} \sim \sum_{\text{classical}} (\text{amp} \times \text{phase})_{\text{path}} + O(h), \quad (3.35)
$$

where, the sum is over classical paths and the higher order terms are in higher powers of $\hbar$. This is an asymptotic equation. In other words, going to higher powers of $\hbar$ does not necessarily lead to convergence (it seldom does). This

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19I am painfully avoiding using something like $\hbar \to 0$ since this gives the wrong impression that $\hbar$, a fundamental constant of nature, is changing.

20A more detailed analysis will reveal how near should the paths be in this path space for them to contribute. One possible estimate, in one dimensional cases, is that paths which are within order $\sqrt{h}$ of the classical $q(t)$.

21In fact, the so called symplectic geometry is at the heart of all this. So much so that one of the very active workers in this field, Alan Weinstein, calls it the “symplectic creed”.

3.2. SEMICLASSIZING THINGS

you can guess even to begin with since we are dealing with essential singularities here and they cannot be taken care of by doing perturbation theory in \( \hbar \). So, there is an amplitude and a phase associated with each contributing path. The phase part is dimensionless and to keep the dimensions straight we have to have a dimensionfull amplitude factor. Since \( \langle q_2 | q_1 \rangle = \delta(q_2 - q_1) \) has the dimensions of inverse length (why?) so our amplitude term also better have the dimensions of inverse length. One other way of seeing this is that we would like to have a probability density interpretation for things and as the propagator itself obeys the Schroedinger equation we better have the dimensions of \( \langle q_2 | q_1 \rangle \) equal to length\(^{-1} \) in one dimension. In more than one dimension similar arguments suggest the appropriate dimensions. At this point you should also thumb through second.

Now, the main question is that what are these amplitude and phases for each path. Turns out that both are determined solely by classical dynamics. But let us refine the previous statement on the main contributions to the path integral as follows: What one is claiming here is that the main contribution to the integral comes from the stationary phase points. If there is only one stationary phase point then to a fair approximation the integral is essentially the value of the integrand at that point. However, we have said that this would correspond to the purely classical trajectory. Since we want to include a few “nearby” paths as well, we get the amplitude factor for each such stationary phase point (classical solution). Thus

\[
\langle q_2, t | q_1, 0 \rangle \sim \sum_{sp} A_{sp} \times e^{iS_{sp}/\hbar} + O(\hbar).
\] (3.36)

Here, \( sp \) stands for stationary phase points. Now, I do not really feel like giving the details of the stationary phase approximation. Let me be a bit sloppy to get the basic philosophy across. This is to get a feel for what the amplitude factor should look like. We already know about the phase - it is just the classical action corresponding to a particular classical trajectory. So, consider an integral with a natural small parameter \( \epsilon \). What we want is to evaluate the following integral

\[
I(\epsilon) \equiv \int e^{i f(z)/\epsilon} dz,
\] (3.37)

in the limit as \( \epsilon \to 0 \). Now as argued before if there are no extremum points of \( f(z) \) then the integral is pretty much zero. So, let us assume that there is a extremum point \( \bar{z} \) and thus \( f'(\bar{z}) = 0 \). Since the main contribution comes from \( z \approx \bar{z} \), we expand the function \( f(z) \approx f(\bar{z}) + f''(\bar{z})(z - \bar{z})^2/2 + \ldots \) and retain only the quadratic terms. Thus

\[
I(\epsilon) \approx e^{if(\bar{z})/\epsilon} \int \exp \left[ \frac{i}{2\epsilon} f''(\bar{z})(z - \bar{z})^2 \right] dz
\]
= \left(\frac{2\pi i\epsilon}{f''(\bar{z})}\right)^{1/2} e^{i f(\bar{z})/\epsilon} + O(\epsilon).

(3.38)

The second line is obtained by doing a simple gaussian integral. The fact that higher order corrections are $O(\epsilon)$ can be checked by retaining further terms in the expansion for $f(z)$. This whole thing was assuming only one saddle or stationary phase point $\bar{z}$. In general, if there are a whole bunch of them around say $\bar{z}_s$ then you would just sum over the contribution from every one of the saddle points. So, there it is...the amplitude factor! Notice that for us what would come in the amplitude factor is the second derivative of the classical action with respect to the initial and final positions. Again, I have intentionally not given a more clean derivation but this will have to do for now\(^\text{22}\). Let me just make a few comments about the above stationary phase formula. Firstly, there is no reason to think that the stationary phase points are real. They can be, and are, in general complex. Complex stationary phase points arise very naturally in tunneling systems. Second comment I want to make is about the problems that might arise when more then one of the extremum points are around. You see, essentially we have been doing second order corrections keeping in mind the geometric picture of a gaussian profile around the points of interest. This region has a certain width. Now, if more then one of these points “collide” \textit{i.e.}, they are too close for comfort, then things have to be modified. This leads to the so called \textit{uniformization} techniques. I will not describe these but you can find a readable account, for example, in Child’s book\(^\text{23}\). The third important observation has to do with the square root function. Thinking of $z$ as a dynamical variable (which is true as you will see below) what happens when $f''(z)$ becomes zero or negative? From a mathematical point of view one has to specify the branch of the square root that one has to pick consistent with the dynamics. In general, for many dimensional cases, this can be quite a problem by itself. However, this has been solved by Maslov in a very elegant fashion and Gutzwiller’s work has also shown us the way. After all the things are done properly, essentially a phase factor comes about (read more on this in \textit{7}) which is nontrivial\(^\text{24}\). So now it is reasonable that I show you the semiclassical approximation for the

\(^{22}\)A more rigorous derivation will make clear the orders, corrections and also the multi-dimensional generalizations etc.

\(^{23}\)Strictly speaking you should consult Dingle’s book titled \textit{Asymptotic Expansions} for the real details.

\(^{24}\)This phase factor, called as the Maslov index is not ignorable. In particular it gives the correct quantization conditions. The zero point energy of a harmonic oscillator comes about from this phase! Unfortunately, I cannot provide more detail here since that will take us too far. Again a lot of the beautiful phase space geometry comes in here and in fact the Maslov index is a \textit{topological invariant}. 
3.2. SEMICLASSIZING THINGS

propagator in full glory. Here it is:

\[
\langle q_2, t | q_1, 0 \rangle_{sc} \sim \left( \frac{1}{2\pi i\hbar} \right)^{d/2} \sum_b \left| \text{Det} \left( \frac{\partial^2 S_b(q_2, q_1; t)}{\partial q_2 \partial q_1} \right) \right|^{1/2} \\
\times \exp \left( i S_b(q_2, q_1; t) - \frac{i\pi \mu_b}{2} \right). \quad (3.39)
\]

Here, I have shown the full multidimensional case and the label \( b \) indicates the \( b^{th} \) classical trajectory (corresponds to the \( b^{th} \) stationary phase point). The Maslov index is indicated by \( \mu_b \). The amplitude factor appearing here is in fact a measure of the “stability” of a classical trajectory. This can be seen easily if one remembers the fact that (since action is a generating function) \( \partial_{q_1} S(q_2, q_1; t) = p_1 \). Thus the amplitude factor can be written in terms of \( \partial_{p_1} q_2 \). This is nothing but a measure of stability since we are asking how does the final position vary as the initial momentum is changed. As you might know, the chaotic or non-chaotic nature of the trajectory is manifested in this factor. The whole business of Liapunov exponents comes in here! You can read a little about it in \( ♭ \). The important thing to realize is that in the semiclassical expression for the propagator, everything can be constructed from classical dynamics alone. I will tell you a bit more about the stability matrix down the road. Before ending this discussion let me point out a sticky issue. There is a sum over many possible trajectories which arise due to the double ended boundary conditions. Now, in more then one dimensions this can be a very difficult task to solve for such “root” trajectories. The nonlinearity of classical dynamics makes it hard to do usefull, believable approximations for this root search problem. One way to get around the problem (not solve it or ignore it though!) is suggested by classical canonical transformation theory itself. We know that a classical trajectory with definite initial conditions in phase space is unique. So, let us transform to the so called initial value representation and get rid of the summation over trajectories! In fact if we transform, at fixed \( q_1, t \), from \( q_2 \rightarrow p_1 \) then one can show (try it!) that:

\[
\sum_b dq_2 \rightarrow \left| \frac{\partial q_2(q_1, p_1; t)}{\partial p_1} \right| dp_1. \quad (3.40)
\]

Also noting that \( \partial_{q_1} S(q_2, q_1; t) = -p_1 \) we can write our propagator for one dimensional case in the initial value representation as

\[
\langle q_2, t | q_1 \rangle_{sc} \approx (2\pi i\hbar)^{-1/2} \left| \frac{\partial q_2(q_1, p_1; t)}{\partial p_1} \right|^{1/2} \exp \left( \frac{i S(q_1, q_2(q_1, p_1; t); t)}{\hbar} - \frac{i\pi \mu}{2} \right). \quad (3.41)
\]
Note that now, in trying to go around the root search problem, we have to run a lot more classical trajectories...maybe some initial conditions do not even contribute! Conservation of effort/difficulty is a hard principle to find exceptions for!

You should at this point work out for yourself the case of free particle and the harmonic oscillator. The free particle case is simple but the harmonic oscillator case needs some work. The reason I am asking you to do this is because the semiclassical approximation is exact in these situations and they also serve as useful models in many systems. Many more things can be said at this juncture but let us move on to some applications!

### 3.2.1 Comment

Note the useful operator identity connecting the energy Green’s function and the propagator. As you can anticipate, they must be related by some kind of fourier transform. The exact relation is as follows:

\[ G^+(E) = \frac{1}{i\hbar} \int_0^\infty dt \exp\left( \frac{it}{\hbar}(E - H) \right), \tag{3.42} \]

where the superscript on the energy Green’s function is to remind that \( t \geq 0 \). It is clear that once you have the propagator then energy domain information can be obtained as well from the above relation. From a quantum mechanical point of view, both time and energy representations give you the same amount of information and clearly observables are representation independent. Once you do a semiclassical approximation the duality is spoilt. In other words, with a semiclassical approximation for the propagator if a fourier transform is performed exactly then what you obtain is not the semiclassical approximation of \( G(E) \). So, what is going on here? Is this bad? By the way this is not just for these two representations. If you, for example, make a semiclassical approximation for the wavefunction in coordinate space and then perform a fourier transform on it you will not obtain, in general, the semiclassical counterpart of the momentum space wavfunction. So, if we insist upon such neat dualities then what is the thing that will make everything consistent. Turns out it is the stationary phase approximation itself. Well, you could have anticipated it to begin with since these transforms involve something like \( e^{(\cdot)/\hbar} \) and we are only keeping things to some order in \( \hbar \). Thus, if one takes a semiclassical object in one space and needs to go to the corresponding semiclassical approximation in the dual (or conjugate) space then you need to evaluate the fourier transform also by the stationary phase method. This can be summarized in the following pictorial way:
Here SPFT stands for stationary phase fourier transform. This stationary phase requirement thus is needed to keep things consistent to a given order in $\hbar$.

But now comes the real bright idea due to Heller. It really takes this consistency thing and turns it upside down! So, ok things are consistent if you do all semiclassical manoeuvres by stationary phase. If you do not then the problems start - or do they? Thinking in a different way, what one is saying is that the semiclassical approximations in time representation and energy representation have different accuracies depending on the system parameters. For example, if you have a system which is nearly harmonic oscillator like then the time representation might be a better one to work semiclassically since semiclassical propagator is exact for a harmonic oscillator. The energy Green’s function semiclassically is not exact! So, if you do want information in the energy domain you start by doing the semiclassical approximation in the time domain and then do an exact fourier transform. Thus this lack of consistency thing can be turned into an advantage. Of, course I am avoiding the issue of what harms can be done due to this very lack of consistency - this is a subtle one. One of the things that can happen (I do not have a good proof/argument for this yet!) is that observables can start depending on parameters in your system that in reality it should not. In all sincerity, this is a bit dangerous. Afterall, already semiclassics is asymptotic and on top of this we are proposing to do uncontrollable theory! To get an idea of how much things get out of hand one tests it out on some simple systems. This is what has been done since this idea came about in 1991 and the results have been surprising\textsuperscript{25}.

\textsuperscript{25}Here I should mention, although not comparing by any means, a similar situation regarding the celebrated linear response theory. At first guess you do not really think that it would work all that well. But years of applications have revealed that linear response theory works better in most situations then you would have anticipated. Honestly, very recently (Miller et al. JCP, 109, 4190 (1998)) have observed that “linearized” semiclassical approaches work rather well. So, this analogy with linear response theory is perhaps not all that bad! The story is beginning to get interesting.
CHAPTER 3. SEMICLASSICAL PROPAGATORS - SOME PERSPECTIVES
Chapter 4

Miller’s semiclassical algebra

In the last lecture we saw the key elements of Dirac’s idea wherein you associate a classical canonical transformation \((p, q) \rightarrow (P, Q)\) with quantum unitary transformation. To summarize

\[
F(q, Q) \longleftrightarrow \exp \left[ \frac{i}{\hbar} F(q, Q) \right] \tag{4.1}
\]

Specifically, the quantum transformation element

\[
\langle q | Q \rangle = a(q, Q) \exp \left[ \frac{i}{\hbar} F(q, Q) \right] \tag{4.2}
\]

with \(a(q, Q)\) being the amplitude factor. As Miller points out in his influential advances in chemical physics article (Adv. Chem. Phys. 25, 69, 1974), in classical mechanics the generating functions act as intermediaries but it is in quantum mechanics that they take on a more prominent role: as phases and therefore central to the quantum interference itself. Feynman, in what is now known as the path integral formulation of quantum mechanics, took the above suggestion of Dirac to completion. We could, again, take the path integral approach and decipher the amplitude in the required limit. However, Miller’s approach is very elegant and very much along the Dirac line of thought. Moreover, as Littlejohn puts it, Miller shows the essential covariance of semiclassical mechanics under classical canonical transformations. Consequently, there is an elegant geometrical insight into the Miller

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1The Poisson bracket is invariant under a canonical transformation. So, for example in the lecture when we transformed the one dimensional harmonic oscillator to action-angle variables \((J, \theta)\) then you can show that \(\{\theta(q, p), J(q, p)\}_{q,p} = 1\). This ensures that the classical dynamics doesn’t change under the transformation. Due to classical-quantum correspondence between canonical and unitary transformations, analogous things can be stated for the quantum commutator bracket.
semiclassical algebra. I will not be able to show you this beautiful insight but, you should consult papers by Littlejohn to learn more.

Ok, let me turn to the main questions: What is the amplitude factor? Is that also classically obtainable? In order to obtain \( a(q,Q) \) one first starts by noting that the fundamental transformation element between canonically conjugate quantities:

\[
\langle q | p \rangle = \frac{1}{\sqrt{2\pi i\hbar}} e^{iqp/\hbar} \\
\langle p | q \rangle = \frac{1}{\sqrt{-2\pi i\hbar}} e^{-ipq/\hbar} 
\]

which is equivalent to the fundamental commutation relation \([\hat{q},\hat{p}] = i\hbar\). (Show this!) Therefore no violations of the uncertainty principle are going to arise in the semiclassical dynamics. That is good, incidentally you will also not have issues of zero-point energy violations either. Now, in classical mechanics the two generating functions \( F(q,Q) \) and \( G(p,Q) \) are connected via a Legendre transform

\[
F(p,Q) = qp + G(q,Q) 
\]

In quantum land these types of relations will emerge from the phase of unitary transformations. At the quantum level note the following identity:

\[
\langle q | Q \rangle = \int dp \langle q | p \rangle \langle p | Q \rangle 
\]

Remember, logarithm of products is the sum of logarithms..if you compare the quantum and classical equations above, it is not very hard to imagine that the above quantum identity is nothing but the Legendre transform! If you recollect your thermodynamics you will notice the similarities - Legendre transforms between free energies, Maxwell’s relations and the logical consistency of it all.

Let us see what we can do with the above “quantum Legendre transform”. In fact we will use a different, but equivalent, version:

\[
\langle p | Q \rangle = \int dq \langle p | q \rangle \langle q | Q \rangle 
\]

In the semiclassical limit I can write:

\[
b(p,Q) \exp \left[ \frac{i}{\hbar} G(p,Q) \right] = \int dq \frac{1}{\sqrt{-2\pi i\hbar}} e^{-ipq/\hbar} a(q,Q) \exp \left[ \frac{i}{\hbar} F(q,Q) \right] 
\]

As it stands, the above integral cannot be evaluated. But we are in the semiclassical limit and therefore the stationary phase approximation can be
invoked. In the previous set of notes I have given you some idea about the stationary phase method and hence will not repeat them here. The condition for stationary phase in the above integral is

$$\frac{\partial}{\partial q} \left[ -qp + F(q, Q) \right]_{q=q_s} = 0$$

(4.8)

which is nothing but the classical generating function identity

$$\left[ \frac{\partial F}{\partial q} \right]_{q_s} = p$$

(4.9)

And that is good, since we are in the semiclassical limit. Evaluating the integral by stationary phase we get:

$$b(p, Q) \exp \left[ \frac{i}{\hbar} G(p, Q) \right] = \frac{1}{\sqrt{-2\pi i \hbar}} \left[ \frac{2\pi i \hbar}{\partial_{qq} F(q, Q)} \right]_{q_s}^{1/2} a(q_s, Q) \exp \left[ \frac{i}{\hbar} (-pq_s + F(q_s, Q)) \right]$$

(4.10)

where $\partial_{qq} F$ denotes the second partial derivative of $F$. At this stage we can compare the RHS and LHS of the above equation to relate the amplitudes and the phases. As you can check easily one gets

$$G(p, Q) = -pq_s + F(q_s, Q)$$

$$b(p, Q) = a(q_s, Q) \left[ -\frac{\partial^2 F(q, Q)}{\partial q^2} \right]_{q_s}^{-1/2}$$

(4.11)

The first one is nothing but the Legendre transform and you should not be surprised by that - we anticipated this! The second one is quite useful and tells us as to how the amplitudes $a(q, Q)$ and $b(p, Q)$ are related. By the way, given the classical generating function relations we see that

$$\frac{\partial^2 F(q, Q)}{\partial q^2} = \frac{\partial p(q, Q)}{\partial q}$$

(4.12)

and you can see the geometrical notion of tangents and envelopes that go with the Legendre transforms. For instance the relation between the two amplitudes gets into trouble when $\partial p(q, Q)/\partial q = \infty$ i.e., points at which the tangent to the $p(q, Q)$ curve is vertical and one cannot disentangle the generating function relations to effect the canonical transformation! Of course there is no need to despair since other generating functions can save the day.

Now that we have one relation, we will use another identity

$$\langle p | q \rangle = \int dQ \langle p | Q \rangle \langle Q | q \rangle$$

(4.13)
Before proceeding with this one let me say that the above is not anything new...especially if I write it is
\[ \langle q | p \rangle^* = \int dQ \langle p | Q \rangle \langle q | Q \rangle^* \] (4.14)
you can, hopefully, see it as essentially the Fourier version of the previous identity that we started out with! I am pointing these things out with the hope that you will appreciate these beautiful things. Allright, now let us get to the job at hand. We can write the above as
\[ \frac{1}{\sqrt{-2\pi i h}} e^{-ipq/h} = \int dQ b(p, Q) a^*(q, Q) \exp \left[ \frac{i}{\hbar} (G(p, Q) - F(q, Q)) \right] \] (4.15)
As before, we can perform the integral using stationary phase method and the condition is
\[ \frac{\partial}{\partial Q} [G(p, Q) - F(q, Q)]_{Q_s} = 0 \] (4.16)
The above is an identity since classically \( \partial_Q F = -P = \partial_Q G \). Hence,
\[ \frac{1}{\sqrt{-2\pi i h}} e^{-ipq/h} = \left[ \frac{2\pi i h}{\partial_Q Q(G(p, Q) - F(q, Q))} \right]^{1/2}_{Q_s} \times b(p, Q_s) a^*(q, Q_s) \exp \left[ \frac{i}{\hbar} (G(p, Q_s) - F(q, Q_s)) \right] \] (4.18)
We can now compare the amplitudes and phase on the LHS and RHS to get
\[ -qp = G(p, Q_s) - F(q, Q_s) \]
\[ \frac{1}{\sqrt{-2\pi i h}} = \left[ \frac{2\pi i h}{\partial_Q Q(G(p, Q) - F(q, Q))} \right]^{1/2}_{Q_s} b(p, Q_s) a^*(q, Q_s) \] (4.19)
The first relation is the classical Legendre transform again..now obeyed at the stationary point in \( Q \) (previously it was at \( q \)..so that is very nice..We have everything consistent in the regions wherein the main contributions to the integrals come from. Thus, there is no need to carry around the stationary point tags like \( q_s, Q_s \) etc. The second one is a relation between the two amplitudes \( a(q, Q) \) and \( b(p, Q) \). One can use the earlier, independent, relation to get
\[ |a(q, Q)|^2 = \frac{1}{2\pi h} \left[ -\frac{\partial^2 F(q, Q)}{\partial q^2} \right]^{1/2} \left[ \frac{\partial^2 G(p, Q)}{\partial Q^2} - \frac{\partial^2 F(q, Q)}{\partial Q^2} \right]^{1/2} \] (4.20)
The above is still not very nice since, seemingly, the amplitude factor for the \( \langle q | Q \rangle \) transformation involves the generator for the \( \langle p | Q \rangle \) transformation!
This can be sorted out by using the Legendre transform relation between the two generators and some nifty implicit differentiations. Let me not do it here and instead refer you to the Miller ACP 1974 article. The final result is that:

\[ |a(q, Q)|^2 = \frac{1}{2\pi\hbar} \frac{\partial^2 F(q, Q)}{\partial q \partial Q} \]  

(4.21)

and therefore the amplitude factor is also completely determined by the classical generating function itself! This, I hope you realize, is amazing and nothing short of a miracle. So, the quantum transformation element is related to the classical canonical generators by

\[ \langle q|Q \rangle = \left[ \frac{1}{-2\pi i\hbar} \frac{\partial^2 F(q, Q)}{\partial q \partial Q} \right]^{1/2} \exp \left[ \frac{i}{\hbar} F(q, Q) \right] \]  

(4.22)

That is the reason that one thinks that

**Classical canonical transf. ~ Quantum unitary transf. +O(\hbar)**

I have been a bit slippery in that I have put in the proper phase factor for the amplitude without giving the derivation - again you can find the clear arguments in Bill’s ACP74 paper.

I will finish this lecture with a physical interpretation. The quantity \( |\langle q|Q \rangle|^2 \), for fixed \( Q \), is nothing but the probability distribution of \( q \). Therefore the identity

\[ |\langle q|Q \rangle|^2 = \frac{1}{2\pi\hbar} \left| \frac{\partial^2 F(q, Q)}{\partial q \partial Q} \right| = \frac{1}{2\pi\hbar} \left| \frac{\partial P(q, Q)}{\partial q} \right| \]  

(4.23)

is consistent with the fact that the

\[ \text{Prob}(P)dP = \text{Prob}(q)dq \]  

(4.24)

with \( \text{Prob}(P) = \text{constant} \) (since \( Q \) is fixed and uncertainty principle says that \( P \) completely uncertain!). Even the constant is identified as \( (2\pi\hbar)^{-1} \) which is correct. Thus, this semiclassical algebra is logically consistent. For details and lots of examples you should consult the ACP74. I hope that I have given you a flavor of things!