Contents

0.1 Feynman's Path Integral Formulation and Lagrangian Mechanics

0.1.1 Mathematical Interlude: Gaussian Integrals

Let us consider the basic Gaussian integral:

$$I = \int_{-\infty}^{\infty} dx\, e^{-ax^2}$$

As it's written this cannot be directly solved but we know a trick:

$$I^2 = \left(\int_{-\infty}^{\infty} dx\, e^{-ax^2}\right)\left(\int_{-\infty}^{\infty} dy\, e^{-ay^2}\right) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\, e^{-a(x^2+y^2)}$$

We then move into polar coordinates:

$$I^2 = \int_0^{\infty}\int_0^{2\pi} rd\phi dr\, e^{-ar^2} = 2\pi \int_0^{\infty} dr\, re^{-ar^2} = 2\pi \left.\frac{-1}{2a}e^{-ar^2}\right|_0^{\infty} = 2\pi\frac{1}{2a} = \frac{\pi}{a}$$

So we conclude:

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\frac{\pi}{a}} \tag{1}$$

Let us now consider a slightly more general integral:

$$\int_{-\infty}^{\infty} dx\, e^{f(x)} = \int_{-\infty}^{\infty} dx\, e^{ax^2+bx+c}$$

Where $f(x)$ is as written simply some quadratic function of x, where specifically we assume it's quadratic coefficient is negative (ie $a < 0$) so the integral converges. To evaluate this we simply complete the square:

$$\begin{aligned}
\int_{-\infty}^{\infty} dx\, e^{-f(x)} &= \int_{-\infty}^{\infty} dx\, e^{ax^2+bx+c} \\
&= \int_{-\infty}^{\infty} dx\, e^{ax^2+bx+\frac{b^2}{4a}-\frac{b^2}{4a}+c} \\
&= \int_{-\infty}^{\infty} dx\, e^{a\left(x+\frac{b}{2a}\right)^2-\frac{b^2}{4a}+c} \\
&= e^{-\frac{b^2}{4a}+c}\int_{-\infty}^{\infty} dx\, e^{a\left(x+\frac{b}{2}\right)^2} \\
&= e^{-\frac{b^2}{4a}+c}\int_{-\infty}^{\infty} du\, e^{au^2} \qquad u = x+\frac{b}{2a} \qquad \& \qquad du = dx \\
&= e^{-\frac{b^2}{4a}+c}\sqrt{\frac{\pi}{-a}}
\end{aligned}$$

Now this exponential prefactor is a bit gross but we can find a nicer form by realizing it's just $f(x)$ evaluated where $\sqrt{a}x + \frac{b}{2\sqrt{a}}$. Now luckily this condition has a more elegant form which can be seen by taking the derivative of $f(x)$ while in it's square completed form:

$$\frac{df}{dx} = 2\left(\sqrt{a}x + \frac{b}{2\sqrt{a}}\right)\sqrt{a}$$

So this prefactor can be more elegantly stated as $f(x)$ evaluated where it's derivate is 0 which I will denote as $f(x)|_{\delta x=0}$. We can also label a more elegantly as $a = \frac{1}{2}\frac{d^2 f}{dx^2}$Thus we conclude:

$$\int_{-\infty}^{\infty} dx\, e^{f(x)} = \sqrt{\frac{2\pi}{-\frac{d^2 f}{dx^2}}}\, e^{\,f(x)|_{\delta x=0}} \tag{2}$$

Now let us consider a different sort of generalization, instead of taking a gaussian integral over a scalar let us do it over a n-D vector (where $A^i{}_j$ is self-adjoint and positive definite for convergence reasons):

$$I = \int Dx\, e^{-x_i A^i{}_j x^j} = \left(\prod_{k=1}^{n}\int_{-\infty}^{\infty} dx_k\right) e^{-x_i A^i{}_j x^j}$$

Where notice the measure $\int Dx = \prod_{k=1}^{n}\int_{-\infty}^{\infty} dx_k$ is an integral over all possible values of our vector (just as previous integrals went over all values of the scalar). As such it can be written explicitly as a product of integrals where each component is integrated over all values. Now since the exponential argument is a scalar we can evaluate it in any basis we like, and similarly since we will integrate over all configurations of the vector it doesn't matter what basis we use. We will then choose the most convenient basis which is the eigen-basis of $A^i{}_j$ in both cases so the integral becomes:

$$I = \left(\prod_{k=1}^{n}\int_{-\infty}^{\infty} dx_k\right) e^{-\sum_{i=1}^{n} a_i (x^i)^2} = \prod_{k=1}^{n}\int_{-\infty}^{\infty} dx_k\, e^{-a_k (x^k)^2} = \prod_{k=1}^{n}\sqrt{\frac{\pi}{a_k}} = \sqrt{\frac{\pi^n}{\prod_{k=1}^{n} a_k}}$$

Now the product of all the eigenvalues of course has a name, it's the determinant of $A^i{}_j$ so we can write:

$$\int Dx\, e^{-x_i A^i{}_j x^j} = \sqrt{\frac{\pi^n}{\det(A)}} \tag{3}$$

Now following the same general program we will consider a general quadratic function of a vector (where now we require $A^i{}_j$ is self-adjoint and negative definite for convergence):

$$\int Dx\, e^{f(x^i)} = \int Dx\, e^{x_i A^i{}_j x^j + B_k x^k + C}$$

We can attack this in much the same way doing something analogous to completing the square:

$$\begin{aligned}
\int Dx\, e^{x_i A^i{}_j x^j + B_k x^k + C} &= \int Dx\, e^{x_i A^i{}_j x^j + B_k x^k + \frac{1}{4}B_l (A^{-1})^l{}_h B^h - \frac{1}{4}B_m (A^{-1})^m{}_n B^n + C} \\
&= \int Dx\, e^{\left(x_i + \frac{1}{2}B_l (A^{-1})^l{}_i\right) A^i{}_j \left(x^j + \frac{1}{2}(A^{-1})^j{}_h B^h\right) - \frac{1}{4}B_m (A^{-1})^m{}_n B^n + C} \\
&= e^{-\frac{1}{4}B_m (A^{-1})^m{}_n B^n + C}\int Dx\, e^{\left(x_i + \frac{1}{2}B_l (A^{-1})^l{}_i\right) A^i{}_j \left(x^j + \frac{1}{2}(A^{-1})^j{}_h B^h\right)} \\
&= e^{-\frac{1}{4}B_m (A^{-1})^m{}_n B^n + C}\int Du\, e^{u_i A^i{}_j u^j} \qquad u^i = x^i + \frac{1}{2}(A^{-1})^i{}_j B^j \qquad \& \qquad Du = Dx \\
&= e^{-\frac{1}{4}B_m (A^{-1})^m{}_n B^n + C}\sqrt{\frac{\pi^n}{\det(-A)}}
\end{aligned}$$

Once again this is a bit ugly but by not is should not be surprising how we make it prettier, we first note:

$$\frac{df}{dx^j} = 2\left(x_i + \frac{1}{2}B_l (A^{-1})^l{}_i\right) A^i{}_j$$

So as before the prefactor is just $f(x)$ evaluated where it's derivative it zero, ie $f(x^i)\big|_{\delta x^i=0}$. Moreover $A^i{}_j = \frac{1}{2}\frac{df}{dx^j dx_i}$ and so we conclude:

$$\int Dx\, e^{f(x^i)} = \sqrt{\frac{(2\pi)^n}{\det\left(-\frac{df}{dx^j dx_i}\right)}}\, e^{\,f(x^k)\big|_{\delta x^k=0}} \tag{4}$$

Where I have used the determinant property $\det(cA) = c^n \det(A)$ to pul the $\frac{1}{2^n}$ out of the determinant.

Now we have gone as far as mathematical rigor can take us and must stray cautiously into the realm of math that is not proven but only motivated to presume the form of a gaussian integral of a functional:

$$\int \mathcal{D}x e^{F[x(t')]} \propto \det\left(\frac{\delta F}{\delta x(t'')dx(t')}\right)^{-\frac{1}{2}} e^{F[x(t')]}\big|_{\delta x=0}$$

Where here the new measure $\mathcal{D}x$ is the natural continuous generalization of Dx that is to say just as Dx integrated over all possible n-long sequences of real numbers $\mathcal{D}x$ integrates over all t-long functions of x. Where by t-long I just means the functions are defined $x(t')$ for $t' \in [0, t]$. The fact that our functions come with an interval should be no stranger to you then our vectors coming with a dimension. We also notice I have completely thrown out the prefactor, this is because it is because it contains a $(2\pi)^\infty$ and thus is horribly diverging. We also have a determinant of what is generically a differential operator which should be interpreted as the (now infinite) product of eigenvalues, which certainly has no guarantee to be finite. We will just have to hope to regularize things later. The exponential argument which requires us to just find the stationary point of a functional is exactly analogous to all the previous cases. Now those practiced in classical mechanics should know the stationary points of a function are described by a differential equation, they are not unique. To uniquely specify them requires boundary conditions. Another way to understand this is to look back at our derivation and notice it relied on the existence of an inverse for our quadratic operator and we know the inverse of a differential operator is it's Greens function which is not unique until boundary conditions are specified. So it's actually true that this continuous gaussian integral also appears non-unique until you specify boundary conditions. This is actually extremely natural to consider boundary conditions an essential ingredient for differential operators, if you try to discretize space and write down a matrix representation of a derivative you will find you're forced to encode your boundary conditions into the matrix so naturally since we are generalizing integrals over matrices we should expect these to be integrals over differential operators accompanied by boundary conditions. For this reason our continuous integral should really be written:

$$\int_{x_1}^{x_2} \mathcal{D}x e^{F[x(t')]} \propto \det\left(\frac{\delta F}{\delta x(t'')dx(t')}\right)^{-\frac{1}{2}} e^{F[x(t')]}\big|_{\delta x=0} \tag{5}$$

Where we are explicitly integrating only over functions that obey the boundary conditions $x(0) = x_1$ and $x(t) = x_2$. This can be thought of as integrating over all possible paths in x-space from x_1 to x_2, for this reason I will often call this type of integral a path integral.

Another thing that warrants pondering is how this picture changes with complex exponentials since they appear so often in quantum mechanics. Since all our derivations were based off of the initial scalar gaussian integral in (1) is suffices to investigate it with a complex argument then immediately generalize our results. It may be tempting to think that we can just take our existing formula and go since it clearly only has problems at $a = 0$ but we know this cannot be the correct approach since obviously for negative a the integral should diverge yet our formula predicts a finite imaginary result (which is also impossible since the integral was purely real). Clearly our analytic continuation has gone wrong somewhere. Let us replace a with the complex number $ai + \epsilon$ and repeat our derivation to see what changes. Clearly the first part where you square the integral and convert to polar coordinates is unaltered, the interesting issue occurs when we try to evaluate the resulting radial integral:

$$I^2 = 2\pi \int_0^\infty dr\, r e^{-(ai+\epsilon)r^2} = 2\pi \frac{-1}{2(ai+\epsilon)} e^{-(ai+\epsilon)r^2}\Big|_0^\infty = \frac{\pi}{ai+\epsilon}\left(1 - e^{-(ai+\epsilon)r^2}\Big|_\infty\right) = \begin{Bmatrix} \frac{\pi}{ai+\epsilon} & \epsilon > 0 \\ \infty & \epsilon < 0 \end{Bmatrix}$$

Where the split in the solution at the end occurs because when ϵ is positive the exponential decays at large values of r leading to the nice familiar formula and when ϵ is negative the exponential explodes at large r and the integral clearly diverges. This leaves us with the following generalized result:

$$\int_{-\infty}^{\infty} dx e^{-zx^2} = \begin{Bmatrix} \sqrt{\frac{\pi}{z}} & \Re(z) < 0 \\ \infty & \Re(z) > 0 \end{Bmatrix} \tag{6}$$

This result then immediately propagated down through all our work generalizing all the gaussian integrals we've discussed into the complex plane. One question we might ask is what about purely complex exponentials where the real part is 0. With the methods we've used so far it seems we can't make a determination since the limits from the left and right sides do not match yet if we think a little bit there is a way forward. Consider what sort of function e^{iax^2} is, it's like an oscillatory function e^{ikx} where the frequency of oscillations in x-space is $k = ax$, which is linear with x itself. This means our function is an oscillatory function which oscillates very slowly near the origin and very rapidly far from it. This is of course the source of our issues since our current method failed precisely because we could not evaluate $e^{iax^2}|_\infty$. However this picture also maybe gives us intuition that it ought to be calculable since most of the area under the curve should be localized near the origin where it oscillates slowly and the distant regions where it oscillates quickly should average out (just like a real gaussian integral is calculable since the majority of the contribution to the integral is localized to the origin). It seems our function has an oscillating discontinuity at $x = \pm\infty$. Whenever you encounter a situation where your function has some variety of singularity at infinity but it seems that shouldn't contribute to our integral so we will trust our formula for the purely complex case as well.

Generating Functions and Wicks Theorem

Another interesting thing we can do is take moments of our gaussian integrals. The procedure for this is actually quite general so I'll work in terms of a general distribution $P(x)$. The moments of this distribution are defined:

$$\langle x^n \rangle = \int dx P(x) x^n$$

The generating function of these moments is defined:

$$\langle e^{Jx} \rangle = \int dx P(x) e^{Jx} = \int dx P(x) \left(1 + Jx + \frac{1}{2} J^2 x^2 + \cdots + \frac{1}{n!} J^n x^n \right) = \langle 1 \rangle + J \langle x \rangle + \frac{1}{2} J^2 \langle x^2 \rangle + \cdots + \frac{1}{n!} J^n \langle x^n \rangle$$

This is called the generating function because as you can see from the relation above:

$$\frac{\partial^n}{\partial J^n} \langle e^{Jx} \rangle \bigg|_{J=0} = \langle x^n \rangle$$

We will use this extensively, and it will be the basis of perturbation theory and feynman diagrams. We can also use this to write down correlation functions between different components in our vector case, one can readily convince themselves:

$$\langle x^i x^j \rangle = \frac{\partial}{\partial J_i} \frac{\partial}{\partial J_j} \langle e^{J_k x^k} \rangle \bigg|_{J=0}$$

Or of course you could build any complicated correlation function you like by bringing down more powers of some x^n with the appropriate derivatives with respect to J_n. For the specific case of a gaussian integral we know the form of these correlation functions exactly. Let us presume:

$$P(x^i) = e^{-x_n A^n_m x^m + B_k x^k + C}$$

The generating function is then:

$$\langle e^{J_k x^k} \rangle = \int Dx e^{-x_n A^n_m x^m + (B_k + J_k) x^k + C} = e^{-\frac{1}{4}(B_m + J_m)(A^{-1})^m{}_n (B^n J^n) + C} \sqrt{\frac{\pi^n}{\det(-A)}}$$

Therefore:

$$\langle x^i x^j \rangle = (A^{-1})^{ij} e^{-\frac{1}{4} B_m (A^{-1})^m{}_n B^n + C} \sqrt{\frac{\pi^n}{\det(-A)}} = (A^{-1})^{ij} \int Dx P(x) = (A^{-1})^{ij}$$

In fact in general it is straightforward to see every pair of variables in the correlation function will drop down a power of A^{-1} and the result will be a sum over every possible set of pairings. So in general for an even number of variables in the correlation function we have a result known as Wicks Theorem:

$$\langle x_{i_1}, x_{i_2}, \ldots, x_{i_{2n}} \rangle = \sum_{\substack{\text{pariings of} \\ \{i_1, \ldots, i_{2n}\}}} A^{-1}_{i_{k_1} i_{k_2}} \ldots A^{-1}_{i_{k_{2n-1}} i_{k_{2n}}} \tag{7}$$

This result generalizes to the continuous case in the obvious way.

The Case of Complex Integration Variables

Now as a quick exercise one can show for a an integral of a complex number we have:

$$\int_{-\infty}^{\infty} d(z, \overline{z})\, e^{-\overline{z} a z} = \frac{\pi}{a} \tag{8}$$

Where here $dz = dxdy$, $z = x + iy$ is the integral over the whole complex plane, the lack of a square root coming from the fact that the complex case is already 2 so we didn't have to square our integral before solving in polar coordinates. With this the result above immediately generalizes to everything else we've worked out with the appropriate factor of 2 being lost:

$$\int_{-\infty}^{\infty} dz, \overline{z}\, e^{f(z, \overline{z})} = \frac{2\pi}{-\frac{d^2 f}{dz d\overline{z}}} e^{f(x)|_{\delta z = \delta \overline{z} = 0}} \tag{9}$$

$$\int D(z, z^\dagger)\, e^{f(z^i, z_j^\dagger)} = \frac{(2\pi)^n}{\det\left(-\frac{df}{dz^j d\overline{z}_i}\right)} e^{f(x^k, x_l^\dagger)}\Big|_{\delta x^k = \delta x_l^\dagger = 0} \tag{10}$$

$$\int_{x_1}^{x_2} \mathcal{D}(z, \overline{z}) e^{F[z(t'), z^\dagger(t'')]} \propto \det\left(\frac{\delta F}{\delta z(t')\delta z^\dagger(t'')}\right)^{-\frac{1}{2}} e^{F[z(t'), z^\dagger(t'')]}\Big|_{\delta z(t') = \delta z^\dagger(t'') = 0} \tag{11}$$

Wicks Theorem as well has an appropriate complex generalization where the pairs must now be explicitly pairs of z_i and $z_j^\dagger$:

$$\langle z_{i_1}^\dagger, z_{i_2}^\dagger, \ldots, z_{j_n}^\dagger, z_{j_1}, z_{j_2}, \ldots, z_{i_n}\rangle = \sum_P A^{-1}_{j_1 i_{P1}} \ldots A^{-1}_{j_n i_{Pn}} \tag{12}$$

Where $\sum_P$ is a sum over all permutations of n integers.

0.1.2 Propagators and Path Integrals

Let us consider a simple question: You start at time t' with a state $|\Psi, t'\rangle = \int dq \Psi(q, t')\, |q\rangle$ and you want to know what the wave function will be at some future time t. We can derive an expression for this straightforwardly:

$$\Psi(q, t) = \langle q|\Psi, t\rangle = \langle q|e^{-\frac{i}{\hbar}\int_{t'}^{t} dt'' \hat{H}(t'')}|\Psi, t'\rangle = \int dq'\, \langle q|e^{-\frac{i}{\hbar}\int_{t'}^{t} dt'' \hat{H}(t'')}|q'\rangle\, \langle q'|\Psi, t'\rangle$$

So we write:

$$\Psi(q, t) = \int dq' \Psi(q', t') K(q', t', q, t) \qquad \text{Where} \qquad K(q', t', q, t) = \langle q|e^{-\frac{i}{\hbar}\int_{t'}^{t} dt'' \hat{H}(t'')}|q'\rangle \tag{13}$$

$K(q', t', q, t)$ is the so called q-space propagator which can be thought of as the transition amplitude from q' at t' to q at some later time t. A transition amplitude just like a component can be turned into a probability of the transition by taking it's magnitude squared but for determining interference effects and such the actual complex number you have before squaring is also important. You can also think of the propagator as the matrix elements of the time evolution operator in the q-basis, or equivlently the solution to the initial value problem where $\Psi(q', 0) = \delta(q - q')$.

It's clear from (13) that if we know the propagator all time evolution can in principle be computed for any initial conditions so naturally computing the propagator is of great interest. It is worth saying that often computing the propagator for a particular observable's basis will be easy if your hamiltonian is well behaved and none of what I'm about to discuss will be relevant, however there will be times when the procedure I am about to derive will be your only recourse. It of course also provides some insight into the structure of the theory to work through this. We do this by repeated use of the completeness relation of break it into integrals over infinitesimal propagators:

$$\begin{aligned}
K(q', t', q, t) &= \langle q|e^{-\frac{i}{\hbar}\int dt \hat{H}(t)}|q'\rangle \\
&= \lim_{\Delta t\to 0} \langle q|\prod_{j=1}^{N} e^{-\frac{i}{\hbar}\Delta t \hat{H}(t' + j\Delta t)}|q'\rangle \\
&= \lim_{\Delta t\to 0} \int \prod_{j=1}^{N} dq_j\ \langle q'|e^{-\frac{i}{\hbar}\Delta t \hat{H}(t' - \Delta t)}|q_N\rangle\, \langle q'|e^{-\frac{i}{\hbar}\Delta t \hat{H}(t - 2\Delta t)}|q_{N-1}\rangle \ldots \langle q_2|e^{-\frac{i}{\hbar}\Delta t \hat{H}(t' + 2\Delta t)}|q_1\rangle\, \langle q_1|e^{-\frac{i}{\hbar}\Delta t \hat{H}(t' + \Delta t)}|q'\rangle \\
&= \lim_{\Delta t\to 0} \int \prod_{j=0}^{N} dq_j\ \langle q_{j+1}|e^{-\frac{i}{\hbar}\Delta t \hat{H}(t' + j\Delta t)}|q_j\rangle \qquad \text{with} \qquad q_0 = q' \qquad \& \qquad q_{N+1} = q
\end{aligned}$$

We will now for ease relabel $t_j'' = t' + j\Delta t$. Additionally presume our hamiltonian is seperable into a kinetic an potential piece $\hat{H}(\hat{p}, \hat{q}) = \hat{T}(\hat{p}) + \hat{V}(\hat{q})$ so we can invoke the Baker-Campbell-Hausdorff formula:

$$e^{\hat{A}+\hat{B}} = e^{\hat{A}} e^{\hat{B}} \left(1 - \frac{1}{2}\left[\hat{A}, \hat{B}\right] + \ldots\right)$$

So in our case this means:

$$e^{-\frac{i}{\hbar}\Delta t \hat{H}(\hat{q}, \hat{p}, t_j'')} = e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p}, t_j'')} e^{-\frac{i}{\hbar}\Delta t \hat{V}(\hat{q}, t_j'')} \left(1 + \frac{\Delta t^2}{2\hbar^2}\left[\hat{T}(\hat{p}), \hat{V}(\hat{q})\right]\right) \approx e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p}, t_j'')} e^{-\frac{i}{\hbar}\Delta t \hat{V}(\hat{q}, t_j'')}$$

Where clearly the last statement becomes an exact equivalence once we take $\Delta t \to 0$ so we are still deriving an exact formula. We now apply this separation and note we can now evaluate the potential explicitly at a specific q value since it's acting on a q-eigenstate. When I do this I will take the hat of the potential since it is now just a function:

$$K(q',t',q,t) = \lim_{\Delta t \to 0} \int \prod_{j=0}^{N} dq_j \ \langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p},t_j'')} e^{-\frac{i}{\hbar}\Delta t \hat{V}(\hat{q},t_j'')} |q_j\rangle \quad = \lim_{\Delta t \to 0} \int \prod_{j=0}^{N} dq_j \ \langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p},t_j'')} e^{-\frac{i}{\hbar}\Delta t V(q_j,t_j'')} |q_j\rangle$$

We will now use the p-space completion relation to insert a set of p-eigenstates between each pair of positions so for each such pair we have:

$$\langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p},t_j'')} e^{-\frac{i}{\hbar}\Delta t V(q_j,t_j'')} |q_j\rangle = \int dp_j \ \langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p},t_j'')} |p_j\rangle \langle p_j| e^{-\frac{i}{\hbar}\Delta t V(q_j,t_j'')} |q_j\rangle$$

We then note we are now applying $\hat{T}$ directly to a momentum eigenstate so we can evaluate it at the specific p_j. We can then pull these exponentials out front and evaluate the inner products between the q and p eigenstates directly using (**??**) allowing us to write:

$$\begin{aligned}
\int dp_j \ \langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t \hat{T}(\hat{p},t_j'')} |p_j\rangle \langle p_j| e^{-\frac{i}{\hbar}\Delta t V(q_j,t_j'')} |q_j\rangle &= \int dp_j \ \langle q_{j+1}| e^{-\frac{i}{\hbar}\Delta t T(p_j,t_j'')} |p_j\rangle \langle p_j| e^{-\frac{i}{\hbar}\Delta t V(q_j,t_j'')} |q_j\rangle \\
&= \int dp_j \ e^{-\frac{i}{\hbar}\Delta t (T(p_j,t_j'') + V(q_j,t_j''))} \langle q_{j+1}|p_j\rangle \langle p_j|q_j\rangle \\
&= \int dp_j \ e^{-\frac{i}{\hbar}\Delta t H(p_j,t_j'')} \frac{1}{2\pi\hbar} e^{\frac{i}{\hbar} p_j (q_{j+1}-q_j)}
\end{aligned}$$

We then plug this back in and define $\dot{q}_j = \frac{q_{j+1}-q_j}{\Delta t}$:

$$K(q',t',q,t) = \lim_{\Delta t \to 0} \int \prod_{j=1}^{N} \frac{dq_j \, dp_j}{2\pi\hbar} \, e^{\frac{i}{\hbar}\Delta t \left(p_j \dot{q}_j - H(q_j,p_j,t_j'')\right)} = \lim_{\Delta t \to 0} \left(\int \prod_{j=1}^{N} \frac{dq_j \, dp_j}{2\pi\hbar} \right) e^{\frac{i}{\hbar}\sum_{j=1}^{N} \Delta t \left(p_j \dot{q}_j - H(q_j,p_j,t_j'')\right)} \tag{14}$$

We will now take the continuum limit. We note when we do this we acquire a prefactor of $(2\pi\hbar)^{-\infty}$ since $N = \frac{t}{\Delta t}$. This sort of anti-divergence suppressing our propagator by something to a negative infinite power is exactly what regulates the divergence typical of these path integrals where the prefactor looks like something to an infinite power. Carefully computing the propagator this way directly would require us to keep everything discrete and only that the continuum limit when the calculation is over and all the prefactors have canceled their diverging bits. Thats quite laborious so instead we will drop the prefactor and be content to with a proportionality. It will become clear later this is often enough as we have other regulatory schemes we can use to get prefactors. We now to write:

$$K(q',t',q,t) \propto \int_{q',p'}^{q,p} \mathcal{D}q\mathcal{D}p \, e^{\frac{i}{\hbar}\int_{t'}^{t} p\dot{q} - H(q,p,t'')dt''} \tag{15}$$

Now notice something miraculous has occurred, the argument of our exponential is the action in the hamiltonian formalism, since we've found an action lagrangian mechanics must be close at hand. We know the lagrangian formalism contains no p dependence so the natural thing to do is to integrate over p.

Here we make a key physical assumption. We **assume** that the hamiltonian is no more than quadratic in p such that we can perform a gaussian integral. If this is not true for a specific system you would have to stop here and work with the path integral over phase space directly.

Taking this gaussian integral we of course arrive at:

$$K(q',t',q,t) \propto \int \mathcal{D}q \, e^{\frac{i}{\hbar}\int_{t'}^{t} p\dot{q} - H(q,p,t'')dt''}\Big|_{\delta p = 0}$$

Here I have neglected the prefactor out front (which for a typical hamiltonian would be the determinant of the laplacian) since I only seek a proportionality and will regularize the lagrangian path integral directly when the time comes. The stationary condition of the argument can be read off as:

$$\dot{q} - \frac{\partial H(q,p,t)}{\partial p} = 0 \qquad \Rightarrow \qquad \dot{q} = \frac{\partial H(q,p,t)}{\partial p}$$

This is of course precisely one of Hamiltons equations. We know our new exponential can be written without p dependence since we've integrated it out, so when the condition above holds we have:

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

So we see that integrating out p is exactly the Legendre transform of classical mechanics and we can write out q-space path integral in terms of the lagrangian directly:

$$K(q', t', q, t) \propto \int_{q'}^{q} \mathcal{D}q \, e^{\frac{i}{\hbar}\int_{t'}^{t} L(q,\dot{q},t'')dt''} = \int \mathcal{D}q \, e^{\frac{i}{\hbar}S} \tag{16}$$

For a general lagrangian this is as far as we can go exactly however we can certainly approximate any propagator by expanding it about it's stationary points (classical paths) to second order then evaluating the resulting gaussian integrals. We might even go so far as to expect this to be a good approximation since presuming the action is polynomial in our coordinates the exponential of it should be strongly peaked about such gaussian points. If you're unconvinced I recommend you use this scheme to approximate an integral representation of the Gamma function to get an approximate formula for factorials, you should arrive at sterlings approximation which is famously very good.

0.1.3 Regularizing Propagators and Wick Rotations

Now a key feature of any path integral calculation is a calculation which did not involve a path integral and thus can be known even up to prefactors. The most obvious such grounding calculation is that of a free field theory:

$$\begin{aligned}
K_{Free}(q', t', q, t) &= \langle q| e^{-\frac{i}{\hbar}(t'-t)\frac{\hat{p}^2}{2m}} |q'\rangle \\
&= \int dp \, \langle q| e^{-\frac{i}{\hbar}(t'-t)\frac{\hat{p}^2}{2m}} |p\rangle \, \langle p|q'\rangle \\
&= \int dp e^{-\frac{i}{\hbar}(t'-t)\frac{p^2}{2m}} \, \langle q|p\rangle \, \langle p|q'\rangle \\
&= \frac{1}{2\pi\hbar}\int dp e^{-\frac{i}{\hbar}(t'-t)\frac{p^2}{2m}} e^{\frac{i}{\hbar}p(q-q')} \\
&= \sqrt{\frac{m}{2\pi i\hbar(t-t')}} \exp\left(\frac{i}{\hbar}\frac{m(q-q')^2}{2(t-t')}\right)
\end{aligned}$$

This result will be a useful to conceptually tether ourselves to later and deduce prefactors by requiring we match it in the appropriate free field limit. As an example of this lets compute the propagator for a simple harmonic oscillator. For simplicity we'll let the initial time be 0 and we will study the transition from the bottom of the well to the bottom of the well. In other words we study just the oscillations around the bottom of the well. Specifically we expand around the static classical solution, we neglect the solutions which oscillate once and return since they only exist at certain exact times and thus can't effect the general function since they don't influence infinitesimally nearby times:

$$
\begin{aligned}
K_{SHO}(0,0,0,t) &\propto \int \mathcal{D}q \exp\left(-\frac{i}{\hbar}\frac{m}{2}\int_0^t dtq\left(\partial_t^2+\omega^2\right)q\right)\\
&\propto \det\left(-\frac{m}{2}\left(\partial_t^2+\omega^2\right)\right)^{-\frac{1}{2}}\exp\left(\frac{i}{\hbar}\cancelto{0}{S_{\text{cl}}}\right)\\
&\propto \prod_{n=1}^{\infty}\left(-\frac{m}{2}\left(\left(\frac{n\pi}{t}\right)^2+\omega^2\right)\right)^{-\frac{1}{2}}\\
&\propto \prod_{n=1}^{\infty}\left(\frac{-\frac{m}{2}\left(\left(\frac{n\pi}{t}\right)^2+\omega^2\right)}{-\frac{m}{2}\left(\frac{n\pi}{t}\right)^2}\left(-\frac{m}{2}\left(\frac{n\pi}{t}\right)^2\right)\right)^{-\frac{1}{2}}\\
&\propto \left[\prod_{n=1}^{\infty}\left(1+\left(\frac{\omega t}{n\pi}\right)^2\right)^{-\frac{1}{2}}\right]\prod_{n=1}^{\infty}\left(-\frac{m}{2}\left(\frac{n\pi}{t}\right)^2\right)^{-\frac{1}{2}}\\
&= \left[\prod_{n=1}^{\infty}\left(1+\left(\frac{\omega t}{n\pi}\right)^2\right)^{-\frac{1}{2}}\right]K_{Free}(0,0,0,t)\\
&= \left[\frac{\omega t}{\sin(\omega t)}\right]^{\frac{1}{2}}\sqrt{\frac{m}{2\pi i\hbar t}}\\
&= \left[\frac{m\omega}{2\pi i\hbar\sin(\omega t)}\right]^{\frac{1}{2}}
\end{aligned}
$$

From this we already see some nice physics, if I measure a particle to be very localized to the bottom of the well then my propagator is basically my state vector in the q-basis at some later time. So what we've calculated is the probability density of such a particle near the bottom of the well as function of time. We see clearly that it diverges whenever $t = \frac{n\pi}{\omega}$ indicating we're certain to keep measuring the particle at the bottom of the well if we space our measurements our by a multiple of a half period exactly as one would expect. Alternatively we see the particle's state is least concentrated near the bottom of the well a quarter cycle off from those times exactly as expected. At least all this is exactly as expected for an oscillating solution, yet we studied the classical static solution. This shows us some important phenomenology, even if we study the classical static solution the quantum theory still has some oscillations, so it seems quantum fluctuations are unavoidable.

Now lets turn to a slightly more involved example, consider two nearby wells symmetrically distributed at $\pm a$ in q-space. We wish to evaluate the survival/tunneling probabilities so we'd like to evaluate the propagator:

$$K(a,0,\pm a,t) \propto \int \mathcal{D}q \exp\left(\frac{i}{\hbar}\int_0^t dt\frac{m}{2}\dot{q}^2 - V(q)\right)$$

However we have a problem before we can even begin, there is no classical solution here to expand around in which the particle leaps the barrier between our wells. There is however a sly trick we can pull exploiting analyticity of our functions by rotating in the complex plane $\tau = it$ or equivalently $t = -i\tau$ and this $dt^2 = -d\tau^2$, this rotation into complex time is known as a wick rotation. Making this substitution we invert the kinetic energy rendering all kinetic energy negative, pulling the overall sign in front we can think of this like flipping the potential energy. Now our particle does not sit in a well but on a hill and we can expand about the classical path where it roll through the valley and onto the other hill. In terms of our euclidean time the relevant amplitude to transition in some euclidean time τ is:

$$K(a,0,\pm a,\tau) \propto \int \mathcal{D}q \exp\left(-\frac{1}{\hbar}\int_0^\tau d\tau\frac{m}{2}\dot{q}^2 + V(q)\right)$$

We should take a moment to work out the action of this classical path in imaginary time, which is customarily called an instanton. Using energy conservation first we are careful to remember that since $V(q)$ was our real space potential the effective potential in euclidean time is $-V(q)$ so $E = \frac{m}{2}\dot{q}_{cl}^2 - V(q_{cl})$. Letting the initial energy be zero since we are interested in particles sitting at the bottom of the well this gives us $\frac{m}{2}\dot{q}_{cl}^2 = V(q_{cl})$. We can now work out the action straightforwardly:

$$S_{inst} = \int_0^\tau d\tau\frac{m}{2}\dot{q}_{cl}^2 + V(q_{cl}) = \int_0^\tau d\tau m\dot{q}_{cl}^2 = \int_0^\tau d\tau\frac{dq_{cl}}{d\tau}m\dot{q}_{cl} = \int_{-a}^{a} m\dot{q}_{cl} = \int_{-a}^{a}\sqrt{2mV(q_{cl})}$$

So we have S_{inst} fully in terms of the potential and don't have to worry about finding any solutions to the equations of motion. Let us investigate the temporal extent of the instantons for a moment, we know the solutions are usually oscillations with the frequency set by the quadratic term, now rotating to euclidean time those should be real exponentials so we see that our particle should exponentially roll down the hill is a timescale set by the oscillation frequency. For a steeply curved enough well with a high enough barrier this means the instanton is fast compared ot the timescales on which tunneling actually occurs with decent likelihood. We can then imagine there must exist more complex classical solutions which involve a series of instanton/anti-instanton pairs, ie those solutions where the particle bounded between the two mounds a few times. Thus we must consider a sort of ensemble of many instantons and anti-instantons, we term this the instanton gas since it is in many ways like a 1D gas. We also presume the instanton gas is dilute, that most solutions involve instantons far apart and overlapping instantons/anti-instantons are rare. We can then in general write:

$$K(a,0,\pm a,\tau) \approx \sum_{n \text{ even/odd}} K^n \int_0^{\tau} d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n A_n(\tau_1,\ldots,\tau_n)$$

Where $A_n(\tau_1,\ldots,\tau_n)$ is the amplitude associated with n instantons at the specified euclidean times. We know in general $A = A_{cl} \cdot A_q$ where A_{cl} is the exponential of the classical action and $A+q$ is the quantum fluctuations bit which comes from the determinant when we do the gaussian integral. Noting that no action accumulates sitting on the hills we know the classical action associated with this process is simply nS_{inst}. We then know the quantum fluctuations for each interval between instantons, which we already computed before when we studied the fluctuations of a particle in a well. We saw there the fluctuations were the square root of an oscillation so here we expect they are real exponentials of the form:

$$e^{-\omega(\tau_{i+1}-\tau_i)/2}$$

The complete quantum contribution is then:

$$A_q = \prod_{i=0}^{n} e^{-\omega(\tau_{i+1}-\tau_i)/2} = e^{-\tau/2}$$

Note all of this is independent of the τ_i so we then write our propagator:

$$\begin{aligned}
K(a,0,\pm a,\tau) &\approx \sum_{n \text{ even/odd}} K^n e^{-nS_{inst}/\hbar} e^{-\omega\tau/2} \int_0^{\tau} d\tau_1 \int_0^{\tau_1} d\tau_2 \cdots \int_0^{\tau_{n-1}} d\tau_n \\
&= \sum_{n \text{ even/odd}} K^n e^{-nS_{inst}/\hbar} e^{-\omega\tau/2} \frac{\tau^n}{n!} \\
&= e^{-\omega\tau/2} \sum_{n \text{ even/odd}} \frac{1}{n!} \left(K\tau e^{-S_{inst}/\hbar}\right)^n
\end{aligned}$$

So performing the sum:

$$K(a,0,\pm a,\tau) \approx Ce^{-\omega\tau/2} \begin{Bmatrix} \cosh\left(K\tau e^{-S_{inst}/\hbar}\right) \\ \sinh\left(K\tau e^{-S_{inst}/\hbar}\right) \end{Bmatrix}$$

Now before we proceed much further lets do a non-path integral calculation, we know for two completely independent wells the ground states are just the independent ground states in the wells. However for a barrier between them of finite height we know the energy levels split into a symmetric and antisymmetric piece. We then explicitly compute the propagator using the approximate completion relation at low energies:

$$\begin{aligned}
K(a,0,\pm a,\tau) &= \langle a|e^{-\tau H/\hbar}|\pm a\rangle \\
&= \langle a|\left(e^{-\tau\epsilon_S/\hbar}|S\rangle\langle S| + e^{-\tau\epsilon_A/\hbar}|A\rangle\langle A|\right)|\pm a\rangle \\
&= e^{-\tau\epsilon_S/\hbar}\langle a|S\rangle\langle S|\pm a\rangle + e^{-\tau\epsilon_A/\hbar}\langle a|A\rangle\langle A|\pm a\rangle
\end{aligned}$$

By symmetry we know:

$$\langle a|S\rangle = \langle -a|S\rangle \qquad \Rightarrow \qquad \langle a|S\rangle\langle S|\pm a\rangle = |\langle a|S\rangle|^2 = \frac{C}{2}$$

$$\langle a|A\rangle = -\langle -a|A\rangle \qquad \Rightarrow \qquad \langle a|A\rangle\langle A|\pm a\rangle = \mp|\langle a|A\rangle|^2 = \mp\frac{C}{2}$$

Where C is just the normalization of the $|\pm a\rangle$ states which for week coupling we take it's probability to be evenly distributed between the two wells. We can also write these energies as the normal ground state energy of the well plus a small offset so $\epsilon_{A/S} = (\hbar\omega \pm \Delta\epsilon)/2$We then have:

$$\begin{aligned} K(a, 0, \pm a, \tau) &= \frac{C}{2}\left(e^{-\tau(\hbar\omega - \Delta\epsilon)/2\hbar} \mp e^{-\tau(\hbar\omega + \delta\epsilon)/2\hbar}\right) \\ &= Ce^{-\omega\tau/2}\begin{Bmatrix} \cosh\left(\Delta\epsilon\tau/2\hbar\right) \\ \cosh\left(\Delta\epsilon\tau/2\hbar\right) \end{Bmatrix} \end{aligned}$$

So comparing to our path integral we see:

$$\Delta\epsilon = 2\hbar K e^{-S_{inst}/\hbar}$$

Remarkably all that remains is to compute K and we will have discovered the splitting energy between our states from which we can derive anything else we need.