1. Path integrals

Before discussing the path integral approach to quantum mechanics, we first review some features of quantum mechanics. We can separate the fundamentals of quantum mechanics into "kinematics" and "dynamics": The kinematics are everything at a fixed time — Hilbert space, preparation/measurement, probability, observables. The dynamics are the time development. There are several ways to describe time dependence of matrix elements; we will start with a general framework, then specialize.

Time dependence may be associated with either the states (Schrödinger picture) or operators (Heisenberg picture). We will be more explicit at first, taking all the time dependence out of the states and operators and putting it into a "time development operator" $U(t,t')$ that transforms the Hilbert space from time t' (earlier) to time t (later). For example, if we want to relate an earlier state to a later one we evaluate $\langle f|U(t,t')|i\rangle$; more generally, we can look at things like

$$\langle f|...\mathcal{O}_2 U(t_2,t_1)\mathcal{O}_1 U(t_1,t_i)|i\rangle$$

which means to prepare an initial state $|i\rangle$ at time t_i, then act with an operator $\mathcal{O}_1$ at time t_1, operator $\mathcal{O}_2$ at time t_2, etc., and eventually measure the amplitude for a final state $\langle f|$.

Now the dynamics can be described entirely through the properties of U. The general physical properties it must satisfy are

$$\begin{aligned} \textit{causality (locality)}: &\qquad U(t_3,t_2)U(t_2,t_1) = U(t_3,t_1) \\ \textit{unitarity}: &\qquad U(t_2,t_1)^\dagger U(t_2,t_1) = I \end{aligned}$$

Causality tells us that things happen in chronological order: Each event is determined by those immediately preceding. It is a kind of group property; in particular, from considering $t_3 = t_2$ we find that

$$U(t,t) = I$$

We can then write

$$U(t+\epsilon,t) \approx I - i\epsilon H(t)$$

by expanding in ϵ, for some operator $H(t)$ that we call the Hamiltonian. Again applying causality, we find

$$\begin{aligned} \partial_t U(t,t') &= \lim_{\epsilon\to 0} \frac{U(t+\epsilon,t') - U(t,t')}{\epsilon} \\ &= \left(\lim_{\epsilon\to 0} \frac{U(t+\epsilon,t) - I}{\epsilon}\right) U(t,t') = -iH(t)U(t,t') \end{aligned}$$

which is the Schrödinger equation for U. Again applying causality to build up the finite U from products of the infinitesimal ones,

$$U(t_f,t_i) = e^{-i\epsilon H(t_f-\epsilon)}\cdots e^{-i\epsilon H(t_i+\epsilon)}e^{-i\epsilon H(t_i)} \equiv \mathcal{T}\left\{exp\left[-i\int_{t_i}^{t_f} dt\ H(t)\right]\right\}$$

which defines the "time-ordered product" $\mathcal{T}$. Finally, unitarity, another group property, tells us that probability is conserved; in particular, from applying to $U(t+\epsilon,t)$,

$$H(t)^\dagger = H(t)$$

The expression of U in terms of a hermitian Hamiltonian guarantees causality and unitarity. (It "solves" those conditions.) If H is time independent and we have a (orthonormal) basis of eigenstates of H, we can write

$$H|I\rangle = E_I|I\rangle \quad \Rightarrow \quad U(t,t') = \sum_I |I\rangle\langle I|e^{-i(t-t')E_I}$$

In Feynman's path integral approach to quantum mechanics (based on an analogy of Dirac), the action is the starting point for quantization. The basic idea is to begin with the basic quantity in quantum mechanics, the transition amplitude, and write it as an integral of the action

$$\langle f|i\rangle = \int D\phi\ e^{-iS[\phi]}$$

where $\int D\phi$ is a "functional integral": Integrate over $\phi(t)$ for each t (with some appropriate normalization). The boundary conditions in t are defined by the choice of initial and final states. In this subsection we will define this integral in a more explicit way by breaking up the time interval into discrete points and taking the continuum limit; in the next subsection we will study ways to evaluate it using its general properties.

The path integral can be derived from the usual Hamiltonian operator formalism. Considering for simplicity a single coordinate q, the wave function is given in coordinate space by

$$\psi(q) = \langle q|\psi\rangle, \qquad |\psi\rangle = \int \frac{dq}{\sqrt{2\pi}}\,\psi(q)|q\rangle$$

where we use the convenient normalizations

$$\int \frac{dq}{\sqrt{2\pi}}|q\rangle\langle q| = 1 = \int \frac{dp}{\sqrt{2\pi}}|p\rangle\langle p| \quad \left[\langle q|q'\rangle = \sqrt{2\pi}\delta(q-q'),\ \langle p|p'\rangle = \sqrt{2\pi}\delta(p-p')\right]$$

for coordinate and momentum space. To describe time development, we work in the Heisenberg picture, where time dependence is in the operators (and thus their eigenstates):

$$\psi(q,t) = \langle q,t|\psi\rangle$$

Time development is then given completely by the "propagator" or "Green function"

$$G(q_f,t_f;q_i,t_i) \equiv \langle q_f,t_f|q_i,t_i\rangle \quad \Rightarrow \quad \psi(q_f,t_f) = \int \frac{dq_i}{\sqrt{2\pi}}\, G(q_f,t_f;q_i,t_i)\psi(q_i,t_i)$$

Exercise VA1.1

Let's review the relationship between time development in the Heisenberg and Schrödinger pictures. Using the usual relation

$$\langle\psi|Q(t)|\chi\rangle \equiv \langle\psi(t)|Q|\chi(t)\rangle$$

between the time-independent states $|\psi\rangle$ and time-dependent operators $Q(t)$ of the Heisenberg picture and the time-dependent states $|\psi(t)\rangle$ and time-independent operators Q of the Schrödinger picture, define time-dependent eigenstates in two ways:

$$Q|q\rangle = q|q\rangle \quad \Rightarrow \quad \begin{cases} \langle q(t)|\psi(t)\rangle \equiv \langle q|\psi\rangle \\ \psi(q,t) \equiv \langle q|\psi(t)\rangle \equiv \langle q,t|\psi\rangle \end{cases}$$

Given the time development of a state

$$|\psi(t)\rangle = U(t)|\psi\rangle$$

($U(t) \equiv U(t,0)$), find the development of $Q(t)$, $|q(t)\rangle$, and $|q,t\rangle$, and show in particular that $|q(t)\rangle \neq |q,t\rangle$. Which is the eigenstate of $Q(t)$?

In general, even for time-dependent Hamiltonians, we can find the infinitesimal time development explicitly from the definition of the time derivative and the time-dependent Schrödinger equation:

$$[i\partial_t - H(-i\partial_q,q,t)]\langle q,t| = 0$$

$$\Rightarrow \quad \langle q,t+\epsilon| = \langle q,t|\{1 - i\epsilon H[P(t),Q(t),t]\} \approx \langle q,t|e^{-i\epsilon H[P(t),Q(t),t]}$$

and similarly for $\langle p,t+\epsilon|$ (where P and Q are the Hilbert-space operators). To derive the path-integral formalism, we then iterate this result to obtain finite time development by inserting unity infinitely many times, alternating between coordinate and momentum,

$$\langle q_f,t_f|q_i,t_i\rangle = \int \frac{dp_0}{\sqrt{2\pi}}\frac{dq_1}{\sqrt{2\pi}}\frac{dp_1}{\sqrt{2\pi}}\ldots\langle q_f,t_f|\ldots$$

$$...|p_1,t_i+3\epsilon\rangle\langle p_1,t_i+3\epsilon|q_1,t_i+2\epsilon\rangle\langle q_1,t_i+2\epsilon|p_0,t_i+\epsilon\rangle\langle p_0,t_i+\epsilon|q_i,t_i\rangle$$

to obtain successive infinitesimal exponentials,

$$\int \frac{dp_0}{\sqrt{2\pi}}\frac{dq_1}{\sqrt{2\pi}}\frac{dp_1}{\sqrt{2\pi}}...\langle q_f|e^{-i\epsilon H}...e^{-i\epsilon H}|p_1\rangle\langle p_1|e^{-i\epsilon H}|q_1\rangle\langle q_1|e^{-i\epsilon H}|p_0\rangle\langle p_0|e^{-i\epsilon H}|q_i\rangle$$

where the time dependence follows from the previous equation. However, note that all the implicit time dependence of the Heisenberg picture drops out, because we extracted the $e^{-i\epsilon H}$'s, putting all the factors of each matrix element at the same time: Although each matrix element is evaluated at time ϵ earlier than the one to its immediate left, each is of the form

$$\langle a,t+\epsilon|b,t\rangle = \langle a,t|e^{-i\epsilon H[P(t),Q(t),t]}|b,t\rangle = \langle a|e^{-i\epsilon H[P,Q,t]}|b\rangle$$

(where $|b\rangle \equiv |b,t_i\rangle$, etc.), leaving only any explicit time dependence that may appear in the Hamiltonian, effectively translating the other t's $\to t_i$. Then we only need to know

$$\langle q|p\rangle = e^{ipq}, \qquad \langle p|q\rangle = e^{-ipq}$$

to evaluate the matrix elements in the path integral as

$$\int \frac{dp_0}{\sqrt{2\pi}}\frac{dq_1}{\sqrt{2\pi}}\frac{dp_1}{\sqrt{2\pi}}...$$

$$exp\{-i[q_ip_0+\epsilon H(p_0,q_i,t_i)-q_1p_0+\epsilon H(p_0,q_1,t_i+\epsilon)+q_1p_1+\epsilon H(p_1,q_1,t_i+2\epsilon)+...]\}$$

More explicitly, this result is

$$\langle q_f,t_f|q_i,t_i\rangle = \int Dp\ Dq\ e^{-iS}, \qquad Dp\ Dq = \prod_{n=0}^{N-1}\frac{dp_n}{\sqrt{2\pi}}\prod_{n=1}^{N-1}\frac{dq_n}{\sqrt{2\pi}}$$

$$S = \sum_{n=0}^{N-1}\{-(q_{n+1}-q_n)p_n+\epsilon[H(p_n,q_n,t_i+2n\epsilon)+H(p_n,q_{n+1},t_i+(2n+1)\epsilon)]\}$$

$$q_0 = q_i, \quad q_N = q_f; \qquad t_f - t_i = 2N\epsilon$$

Note that by adding (or subtracting) a step or two we could just as well evaluate $\langle q_f,t_f|p_i,t_i\rangle$ or $\langle p_f,t_f|q_i,t_i\rangle$ or $\langle p_f,t_f|p_i,t_i\rangle$.

The classical picture is a segmented path, with the particle traveling along a straight line segment from point q_n to point q_{n+1} with momentum p_n: Each q is associated with a point, while each p is associated with the line segment connecting two consecutive points. In the "continuum" limit $\epsilon \to 0$, $N \to \infty$, $t_f - t_i$ fixed,

$$S = \int_{t_i}^{t_f} dt[-\dot{q}p + H(p,q,t)]$$

(We have dropped some terms in $\langle q|H|p\rangle$ and $\langle p|H|q\rangle$ from reordering the operators Q and P in $H(P,Q)$ to apply $P|p\rangle = p|p\rangle$ and $Q|q\rangle = q|q\rangle$. These commutator terms alternate in sign, combining to give terms of order ϵ^2, and can be dropped in the continuum limit.)

More generally, we can evaluate an arbitrary transition amplitude as

$$\mathcal{A} = \langle f|i\rangle = \int \frac{dq_f}{\sqrt{2\pi}}\frac{dq_i}{\sqrt{2\pi}}\psi_f{}^*(q_f)\langle q_f,t_f|q_i,t_i\rangle\psi_i(q_i) = \int Dp\ Dq\ \psi_f{}^*(q_f)e^{-iS}\psi_i(q_i)$$

where now

$$Dp\ Dq = \prod_{n=0}^{N-1}\frac{dp_n}{\sqrt{2\pi}}\prod_{n=0}^{N}\frac{dq_n}{\sqrt{2\pi}}$$

Note that we can combine the initial and final wave function, as

$$\Psi(q_i,q_f) \equiv \psi_f{}^*(q_f)\psi_i(q_i) \quad \Rightarrow \quad \mathcal{A} = \int Dp\ Dq\ \Psi(q_i,q_f)e^{-iS}$$

The complex conjugation of ψ_f vs. ψ_i is due to the complex conjugation involved in time reversal (as seen, e.g., when comparing an eigenstate of p at the inital time to the same eigenstate at the final time). In field theory, where the "p's and q's" are functions of space as well as time, if we choose the boundary in space also to be finite, so that the space and time boundaries form a single connected and closed boundary, then Ψ is simply a function of the q's over all that boundary.

We now see the relationship of the path integral approach to the time development operator: From the above derivation of the path integral, by integrating back out the insertions of unity immediately after extracting the infinitesimal exponentials and translating the time of each matrix element to zero, we find

$$\langle q,t_f|q,t_i\rangle = \langle q_f|U(t_f,t_i)|q_i\rangle$$

$$U(t_f,t_i) = e^{-i\epsilon H(t_f-\epsilon)}\cdots e^{-i\epsilon H(t_i+\epsilon)}e^{-i\epsilon H(t_i)} = \mathcal{T}\left\{exp\left[-i\int_{t_i}^{t_f}dt\ H(t)\right]\right\}$$

as previously. This is effectively a Schrödinger-picture expression (all the P's and Q's are at the initial time), and can also be derived in that picture by solving for the time dependence of any state $|\psi(t)\rangle$.

2. Semiclassical expansion

The path integral formulation is especially suited for semiclassical approximations: The Bohr-Sommerfeld quantization rule follows from the fact that the functional integral is invariant under $S \to S + 2\pi n$, since S appears only as e^{-iS}; in that sense the action is more like an angle than a single-valued function. The JWKB expansion follows from $S \to S/\hbar$ and expanding in $\hbar$. This expansion can be interpreted as an expansion in (space and time) derivatives, since it leads in the usual way to the identification $p = -i\hbar\partial/\partial x$ and $E = i\hbar\partial/\partial t$.

Exercise VA2.1

For comparison, we review the Schrödinger equation approach. Consider the nonrelativistic JWKB expansion for the propagator (for an arbitrary Hamiltonian H) to the first two orders in $\hbar$, writing it as

$$G \approx \sqrt{\rho} e^{-iS/\hbar}$$

a Show the corresponding orders in the time-dependent Schrödinger equation at $t > 0$ can be written as the classical equation of motion for the action S and the (probability) current conservation law for the (probability) density ρ ("Hamilton-Jacobi equations"),

$$H = \dot{S}, \qquad \frac{\partial}{\partial q^i}\left(\rho \frac{\partial H}{\partial p_i}\right) + \dot{\rho} = 0$$

when the argument p of H is evaluated at

$$p_i = -\frac{\partial S}{\partial q^i}$$

(Assume a symmetric ordering of p's and q's in the quantum H.) Compare the *relativistic* case examined in exercise IIIA4.1.

b The propagator is expressed in terms of q and q_0, where $G(q, q_0, t) \sim \delta(q - q_0)$ at $t = 0$, so the first order in $\hbar$ is found by using the solution to the Hamilton-Jacobi equations to write the classical action in terms of the "final" position q and initial position q_0. (In principle; in general even the classical equations may be too difficult to solve analytically.) However, the Hamiltonian is given as a function of p and q. Show that the change in variables from q, p to q, q_0 gives

$$\frac{\partial H}{\partial p_i} = -(M^{-1})^{ij} \frac{\partial^2 S}{\partial q_0^j \partial t}, \qquad (M)_{ij} = \frac{\partial^2 S}{\partial q_0^i \partial q^j}$$

Show that

$$\rho = det\ (-i\tfrac{1}{\hbar} M)$$

(the "van Vleck determinant") solves the current conservation law, using the explicit expression for $(det\ M)M^{-1}$ given in subsection IB3. Check the normalization, using the initial condition for propagators (or comparing to the free case).

One way to apply the path integral is as follows: (1) Find a classical solution to the equations of motion. This gives the leading contribution in $\hbar$ ("stationary phase approximation"),

$$\int D\phi\ e^{-iS/\hbar} \approx e^{-iS_0/\hbar}$$

(The validity of such an approximation with an imaginary exponent will be discussed in subsection VA5.)

(2) Expand about the classical solution as

$$\phi = \phi_{cl} + \sqrt{\hbar}\Delta\phi$$

Expanding in $\Delta\phi$ (or $\hbar$), we have schematically

$$\hbar^{-1}S = \hbar^{-1}S_0 + \hbar^{-1/2}S_0'\Delta\phi + \tfrac{1}{2}S_0''(\Delta\phi)^2 + \hbar^{1/2}\tfrac{1}{6}S_0'''(\Delta\phi)^3 + ...$$

where "$_0$" means to evaluate at $\phi = \phi_{cl}$ and the derivatives are really functional derivatives (so there is also an integral for each derivative). The first term in the action gives the classical contribution, while the linear term vanishes by the equations of motion. The quadratic term gives an $\hbar$-independent contribution to the exponential, so the next order approximation to the functional integral comes from integrating just that: Integrating Gaussians as in subsection IB3,

$$\int D\phi\ e^{-iS/\hbar} \approx e^{-iS_0/\hbar}(det\ S_0'')^{-1/2}$$

where the determinant is now a functional one, which can be defined by performing the functional integral as in the previous section, as a series of ordinary Gaussian integrals. The boundary conditions are $\Delta\phi = 0$ at t_i and t_f (since $\phi_{cl} = \phi$ there). Normalization constants can be determined by comparing the free case, or considering the limit where the initial and final times converge.

(3) We then expand the exponential in the cubic and higher terms (positive powers of $\hbar$): The resulting functional integral is that of an $\hbar$-independent Gaussian times a polynomial with positive powers of $\hbar$. Since odd orders in $\Delta\phi$ vanish by symmetry ($\Delta\phi \to -\Delta\phi$), only integer powers of $\hbar$ appear:

$$\int D\phi\ e^{-iS/\hbar} = e^{-iS_0/\hbar}\int D(\Delta\phi)e^{-iS_0''(\Delta\phi)^2/2}\left(1 + \sum_{n=1}^{\infty}\hbar^n f_n[\Delta\phi]\right)$$

Polynomials times Gaussians are also straightforward to integrate: The easiest way is to first evaluate integrals of Gaussians with linear terms:

$$\int \frac{d^D x}{(2\pi)^{D/2}} e^{-x^T Sx/2 + j^T x} = (det\ S)^{-1/2} e^{j^T S^{-1} j/2}$$

$$\int \frac{d^D z^*\, d^D z}{(2\pi i)^D} e^{-z^\dagger H z + z^\dagger j + j^\dagger z} = (det\ H)^{-1} e^{j^\dagger H^{-1} j}$$

from shifting the integration variables ($x \to x + S^{-1}j$, etc.) to eliminate the linear terms, then using the previous results. In functions of x multiplying the Gaussian, x can be replaced with $\partial/\partial j$ (and similarly for z) and then pulled outside the integral. (If a linear term is not included, it can be introduced, and the result can be evaluated at $j = 0$.) The final result then takes the form

$$\langle q_f, t_f | q_i, t_i \rangle = e^{-iS_0/\hbar}(A + \hbar B + ...) = exp\left(-i\tfrac{1}{\hbar}\sum_{n=0}^{\infty} \hbar^n S_n\right)$$

Exercise VA2.2

Generalize the above results for integration of Gaussians with linear terms to the cases with fermionic and mixed (subsection IIC3) integration variables.

Exercise VA2.3

Evaluate

$$\int \frac{d^D x}{(2\pi)^{D/2}} e^{-x^T Sx/2} x^i x^j x^k x^l$$

by taking $(\partial/\partial j_i)(\partial/\partial j_j)(\partial/\partial j_k)(\partial/\partial j_l)$ on the above result.

As an example, consider the free nonrelativistic particle. The separability of the action translates into factorization of the functional integral, so the result can be found from the one-dimensional case. As usual,

$$L = -\tfrac{1}{2} m\dot{x}^2 \quad \Rightarrow \quad x_{cl}(t) = x_i + \frac{x_f - x_i}{t_f - t_i}(t - t_i)$$

where we have written the classical solution in terms of the variables appropriate to the initial and final states, namely x_i for an initial state localized there at time t_i, and x_f, t_f for the final state. Since the classical action is itself quadratic, so is its expansion:

$$S = S_{cl} + \Delta S, \qquad S_{cl} = -\tfrac{1}{2} m \frac{(x_f - x_i)^2}{t_f - t_i}, \qquad \Delta S = -\int dt\ \tfrac{1}{2} m(\Delta\dot{x})^2$$

In general, a determinant from the ΔS integral must be evaluated (but see exercise VA2.1). In this simple case, time translation invariance, dimensional analysis, and independence from x_f, x_i are enough to determine the result of that functional integral

up to a constant, fixed by the short-time limit $t_f \to t_i$. The final one-dimensional result is then

$$\langle x_f, t_f | x_i, t_i \rangle = \sqrt{\frac{-im}{t_f - t_i}}\, e^{im(x_f - x_i)^2/2(t_f - t_i)}$$

where we have used

$$\sqrt{2\pi}\delta(x) = \lim_{\epsilon \to 0} \tfrac{1}{\sqrt{\epsilon}} e^{-x^2/2\epsilon}$$

(one way of defining a Dirac δ function) to normalize

$$\langle x_f, t | x_i, t \rangle = \sqrt{2\pi}\delta(x_f - x_i)$$

The Gaussian integral for the free particle can also be performed explicitly, by using the discretized Hamiltonian path integral of the previous subsection.

Exercise VA2.3

The path integral for the free, nonrelativistic particle can be evaluated much more easily using the Hamiltonian form of the action. First consider the Gaussian integral

$$\int_{-\infty}^{\infty} dx\; e^{ipx - \epsilon x^2/2}$$

as a special case of the Gaussians already evaluated, and use it to derive the identity

$$\int_{-\infty}^{\infty} dx\; e^{ipx} = 2\pi\delta(p)$$

(The ϵ thus acts as a regulator to make the integral well defined.) Then use the discretized expression of subsection VA1, and evaluate the x integrals first. All but one of the p integrals then can be trivially evaluated, the last giving a Fourier transform.

Exercise VA2.4

Consider the one-dimensional harmonic oscillator. (The multi-dimesional case is again separable.)

a Explicitly evaluate the discretized path integral to find the result

$$\langle x_f, t_i + t | x_i, t_i \rangle = \sqrt{\frac{-im\omega}{sin\ \omega t}}\; exp\left\{ \frac{im\omega[\frac{1}{2}(x_f^2 + x_i^2)cos\ \omega t - x_f x_i]}{sin\ \omega t} \right\}$$

b Rederive the result using the result of exercise VA2.1. (Hint: First solve the classical equations of motion for $x(t)$, then rewrite it in terms of $x_i = q_0$ and $x_f = q$; plug into $S_{cl} = S$ and apply the above.)

Note that we have been sloppy about the definition of the "integration measure": In going from the Hamiltonian form of the action to the Lagrangian form, we ignored

some m dependence. Specifically, if we start with the Hamiltonian form, as derived in the previous subsection, and derive the Lagrangian form by integrating out p, we find the $1/m$ in $H = p^2/2m$ leads to

$$\prod_{n=0}^{N-1} \frac{dp_n}{\sqrt{2\pi}} \prod_{n=1}^{N-1} \frac{dx_n}{\sqrt{2\pi}} \quad \rightarrow \quad m^{N/2} \prod_{n=1}^{N-1} \frac{dx_n}{\sqrt{2\pi}}$$

The $m^{(N-1)/2}$ then cancels similar factors from the $N-1$ x-integrals, while the remaining $\sqrt{m}$ is that found in the final result above.

If we had considered a more general Hamiltonian, as in subsection IIIA1, where p^2 appeared as $\frac{1}{2}g^{ij}(x)p_ip_j$, then we would have obtained a measure of the form (for $i = 1, ..., D$)

$$[det\ g(x_0) det\ g(x_N)]^{-1/4} \prod_{n=1}^{N-1} \frac{d^D x_n}{(2\pi)^{D/2}\sqrt{det\ g(x_n)}}$$

(We have averaged g as $g(x)p^2 \rightarrow \sqrt{g(x_n)g(x_{n+1})}p_n^2$, since x_n is associated with the point n while p_n is associated with the link from n to $n+1$.) Such measure factors are easy to recognize, since they are always local, without any derivatives: If we included it in the action, it would be a term proportional to

$$ln \prod_n det\ g(x_n) = \tfrac{1}{\epsilon} \sum_n \epsilon\ ln\ det\ g(x_n) \sim \delta(0) \int dt\ ln\ det\ g(x(t))$$

(The factors at x_0 and x_N are for standard normalization of the wave functions, which we can absorb by a redefinition.) In practice we just drop all such factors throughout the calculation, and fix the normalization at the end of the calculation. Since the Lagrangian form follows from the Hamiltonian form, which was properly normalized, we know such factors will cancel anyway. Auxiliary fields can require similar factors for proper normalization; then such factors are simply the Jacobians from the field redefinitions from a form where they appeared with trivial quadratic terms.

3. Propagators

The amplitude we defined by path integration in subsection VA1 is the "propagator" or "Green function" for the Schrödinger equation. Explicitly, we define

$$G(q,t;q',t') \equiv \theta(t-t')\langle q,t|q',t'\rangle$$

where we have included the "step function" $\theta(t-t')$ (1 for $t > t'$, 0 otherwise) to enforce that the final time is later than the initial time (retarded propagator). This satisfies the free case of the general defining equation of the propagator

$$[\partial_t + iH(-i\partial_q, q, t)]G(q,t;q',t') = [-\partial_{t'} + iH(i\partial_{q'}, q', t')]G(q,t;q',t')$$

$$= \sqrt{2\pi}\delta(q-q')\delta(t-t')$$

where we have used

$$\partial_t \theta(t-t') = \delta(t-t')$$

and the facts that G without the θ factor is a homogeneous solution of the Schrödinger equation (no δ's) and becomes a δ in x for small times. The propagator then gives a general solution of the Schrödinger equation as

$$\langle q,t| = \int \frac{dq'}{\sqrt{2\pi}} \langle q,t|q',t'\rangle\langle q',t'| \quad \Rightarrow \quad \psi(q,t) = \int \frac{dq'}{\sqrt{2\pi}} G(q,t;q',t')\psi(q',t')$$

In particular, for $\psi(q,t') = \sqrt{2\pi}\delta(q-q')$ at some time t' for some point q', $\psi(q,t) = G(q,t;q',t')$ at all later times. These equations are matrix elements of the corresponding operator equations; e.g.,

$$G(q,t;q',t') \equiv \langle q|U(t,t')|q'\rangle$$

$$[\partial_t + iH(t)]U(t,t') = U(t,t')[-\overleftarrow{\partial}_{t'} + iH(t')] = \delta(t-t')I$$

where we now include a step function in the definition of the time development operator U:

$$U(t,t') \equiv \theta(t-t')\mathcal{T}\left\{exp\left[-i\int_{t'}^{t} dt\ H(t)\right]\right\}$$

This solution for the propagator is not unique; as usual, a first-order differential equation needs one boundary condition. Another way to say it is that the inhomogeneous differential equation is arbitrary up to a solution of the homogeneous equation. We have eliminated the ambiguity by requiring that the propagator be retarded, as incorporated in the factor $\theta(t-t')$; using instead $-\theta(t'-t)$ would give the advanced propagator.

This has an interesting translation in terms of the Fourier transform with respect to the time, which replaces the so-called "time-dependent" Schrödinger equation with the "time-independent" one. Fourier transforms are a useful way to solve differential equations when performed with respect to variables with translational invariance, since this implies conservation of the conjugate variable: The result is elimination of the corresponding derivatives. In this case, it means the time-independent Schrödinger equation needs a time-independent Hamiltonian. For example, defining

$$\tilde{U}(E,E') \equiv \int \frac{dt}{\sqrt{2\pi}}\frac{dt'}{\sqrt{2\pi}} e^{-i(E't'-Et)}U(t,t')$$

$$\Rightarrow \quad -i(E-H)\tilde{U}(E,E') = \delta(E-E')I$$

$$\Rightarrow \quad \tilde{U}(E,E') = \frac{i}{E-H}\delta(E-E')$$

Now inverse Fourier transforming,

$$U(t,t') = \int \frac{dE}{\sqrt{2\pi}}\frac{dE'}{\sqrt{2\pi}} e^{i(E't'-Et)}\tilde{U}(E,E')$$

$$= \int \frac{dE}{2\pi} e^{-iE(t-t')}\frac{i}{E-H}$$

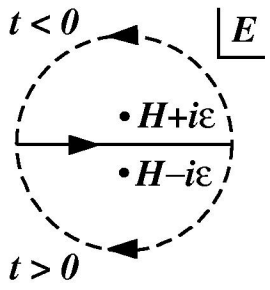
we have an ambiguity in integrating E past the pole at $E=H$. We therefore shift the pole slightly off the real axis, so we can integrate exactly on the real axis. Closing the contour by adding to the real axis a semicircle of infinite radius in either the complex upper- or lower-half-plane, wherever convergent ($\lim_{|t|\to\infty} e^{-|Et|} = 0$, but $\lim_{|t|\to\infty} e^{+|Et|} = \infty$), we find

$$\int \frac{dE}{2\pi} e^{-iEt}\frac{i}{E-H\pm i\epsilon} = \pm\theta(\pm t)e^{-iHt}$$

which gives either the retarded or advanced propagator depending on the choice of sign for the infinitesimal constant ϵ (retarded for $E-H+i\epsilon$). Remember from exercise IIA1.2 that complex integration is essentially just Gauss' law, wth poles acting as charges: The general integral result we used is

$$\oint \frac{dz'}{2\pi i} f(z')\frac{1}{z'-z} = f(z)$$

where the counterclockwise contour of integration encloses the pole at z but no singularity in f, so we can evaluate the integral by Taylor expanding f about z.



To perform the inverse Fourier transform, we note that the exponent needs an infinitesimal negative part to make the integral convergent:

$$\int dt\; e^{iEt}(\pm)\theta(\pm t)e^{-iHt\mp\epsilon t} = \frac{i}{E-H\pm i\epsilon}$$

Exercise VA3.1

Show that

$$\frac{i}{x+i\epsilon}-\frac{i}{x-i\epsilon}=2\pi\delta(x)$$

by three methods:

a Use the above result for the Fourier transform.

b Show that this is the contour integral definition of the δ function, which is actually a distribution, by integration, multiplying by an arbitrary (nonsingular) function and integrating along the real axis. (Hint: Push the poles onto the real axis, shifting the contours along with them, to find the integral of a single function along the difference of two contours.)

c Prove the identity (checking the normalization)

$$\lim_{\epsilon\to 0}\frac{2\epsilon}{x^2+\epsilon^2}=2\pi\delta(x)$$

For the example of the free particle in one dimension we found by various methods

$$G(x,t;x',t')=\theta(t-t')\sqrt{\frac{-im}{t-t'}}\,e^{im(x-x')^2/2(t-t')}$$

However, we could have saved the trouble if we just started in momentum space,

$$\hat{G}(p,t;p',t')\equiv\langle p|U(t,t')|p'\rangle=\langle p|\theta(t-t')e^{-i(t-t')H}|p'\rangle=\theta(t-t')e^{-i(t-t')p^2/2m}\langle p|p'\rangle$$
$$=\theta(t-t')\sqrt{2\pi}\delta(p-p')e^{-i(t-t')p^2/2m}$$

in the retarded case. If we Fourier transform p to x (the same as a change of basis from $|p\rangle$ to $|x\rangle$), the integrals are then simple Gaussians. Again, the result is simpler in p-space because p is conserved. In the relativistic case we will want to treat energy and momentum equally; doing the same here for later comparison, we define

$$\tilde{\psi}(p,E)=\int\frac{dq}{\sqrt{2\pi}}\frac{dt}{\sqrt{2\pi}}e^{-i(qx-Et)}\psi(q,t)$$

and similarly for $\tilde{G}$, and we have

$$\tilde{G}(p,E;p',E')=\frac{i}{E-p^2/2m}\sqrt{2\pi}\delta(p-p')\delta(E-E')$$

4. S-matrices

"Scattering" is defined as a process that starts with a free state and ends with a free state, with interaction (self- or with external forces) at intermediate times, e.g., particles coming in from and going out to spatial infinity and scattering from a

potential of finite spatial extent. Thus, if the interaction is nonvanishing somewhere between times t_1 and t_2, where $t_f > t_2 > t_1 > t_i$, we can write

$$U(t_f, t_i) = U(t_f, t_2)U(t_2, t_1)U(t_1, t_i) = e^{-i(t_f - t_2)H_0}U(t_2, t_1)e^{-i(t_1 - t_i)H_0}$$

in terms of the "free term" H_0 of the Hamiltonian $H = H_0 + H_I$, where H_I is the "interaction term". (H_I may be time dependent, but not H_0.) It is more convenient to work with a quantity that is independent of initial and final times (as long as they are outside of the interaction region t_1 to t_2). We therefore define the "S(cattering)-matrix" operator $\mathcal{S}$ as

$$\mathcal{S} \equiv \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} e^{it_f H_0}U(t_f, t_i)e^{-it_i H_0}$$

where we have thrown in the limit because in the real world interaction doesn't just start and stop, but fades in and out. However, in our simple example above we find

$$\mathcal{S} = e^{it_2 H_0}U(t_2, t_1)e^{-it_1 H_0}$$

In the interacting case, the amplitude we get from the path integral is the interacting propagator. To be able to take the limit describing time development between infinite initial and final times, we need to choose boundary conditions such that the initial and final basis states have the time dependence of free particles, described by H_0, assuming that the particle behaves freely at such asymptotically large times. This is called the "interaction picture", to distinguish from the Heisenberg picture, where the states have no time dependence, and the Schrödinger picture, where the states have the complete interacting time dependence. We thus evaluate the limiting amplitude

$$\mathcal{A} = \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \langle \psi_f(t_f) | \psi_i(t_i) \rangle = \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} \int \frac{dq_f}{\sqrt{2\pi}} \frac{dq_i}{\sqrt{2\pi}} \psi_f{}^*(q_f, t_f) \langle q_f, t_f | q_i, t_i \rangle \psi_i(q_i, t_i)$$

for the interaction-picture states $|\psi(t)\rangle$, relating the interaction-picture coordinate basis ${}_0\langle q, t|$ to the Heisenberg-picture basis $\langle q, t|$ (with initial conditions ${}_0\langle q, 0| = \langle q, 0| \equiv \langle q|$):

$${}_0\langle q, t| = \langle q| e^{-itH_0} \quad \Rightarrow \quad \langle q_f, t_f | q_i, t_i \rangle = {}_0\langle q_f, t_f | e^{it_f H_0}U(t_f, t_i)e^{-it_i H_0} | q_i, t_i \rangle_0$$

$$\psi(q, t) = {}_0\langle q, t | \psi \rangle \quad \Rightarrow \quad \mathcal{A} = \langle \psi_f | \mathcal{S} | \psi_i \rangle$$

with $\mathcal{S}$ as defined above.

The fact that time development conserves probability ($H = H^\dagger$) is reflected in the corresponding *unitarity* condition for the S-matrix:

$$\mathcal{S}^\dagger \mathcal{S} = 1$$

A more complicated condition is *causality*: The basic idea is that interactions take place in chronological order. (A stronger statement of causality will be found in the relativistic case: that any interaction should take place at a spacetime point, rather than just at a single time. It follows from this weaker one in relativistic theories, since event B is later than event A in every Lorentz frame only when B is in A's lightcone.) Causality is the condition that the Hamiltonian at any time involves only variables evaluated at that time. ($H(t)$ is a function of only $\phi(t)$, all at the same time t, where $\phi = p, q$ are the quantum variables appearing in the Hamiltonian.) A nice way to describe the interactions is by introducing a classical background as we did for the semiclassical expansion of path integrals, such as by $\phi(t) \to \phi(t) + \chi(t)$, where χ is just some function. The important point is that we have shifted $\phi(t)$ by $\chi(t)$ at the same t, so as not to disturb causality. We then consider the effect on the S-matrix of modifying the background χ by a function $\delta\chi$ localized (nonvanishing) at some particular time t, and a function $\delta\chi'$ localized at t', such that $t > t'$. Picking out the $\delta\chi$ pieces in the time-ordered product, we can therefore write

$$\mathcal{S}[\chi + \delta\chi + \delta\chi'] = U(f,t)\mathcal{V}(t)U(t,t')\mathcal{V}(t')U(t',i)$$
$$\mathcal{S}[\chi + \delta\chi] = U(f,t)\mathcal{V}(t)U(t,t')U(t',i)$$
$$\mathcal{S}[\chi + \delta\chi'] = U(f,t)U(t,t')\mathcal{V}(t')U(t',i)$$
$$\mathcal{S}[\chi] = U(f,t)U(t,t')U(t',i)$$

where $U(t',i)$ is the time-development operator from time t_i to time t' (including the canceling factor with H_0), $\mathcal{V}(t')$ is the extra factor in the time development at time t' resulting from the function $\delta\chi'$ localized there, etc. Thus we replace a $\mathcal{V}$ with the identity if the corresponding $\delta\chi$ is absent. Then we easily find

$$\mathcal{S}[\chi + \delta\chi + \delta\chi'] = \mathcal{S}[\chi + \delta\chi]\mathcal{S}^{-1}[\chi]\mathcal{S}[\chi + \delta\chi']$$
$$\Rightarrow \quad (\mathcal{S}^{-1}[\chi + \delta\chi]\mathcal{S}[\chi + \delta\chi + \delta\chi'] - I) - (\mathcal{S}^{-1}[\chi]\mathcal{S}[\chi + \delta\chi'] - I) = 0$$
$$\Rightarrow \quad \frac{\delta}{\delta\chi(t)}\left(\mathcal{S}[\chi]^\dagger \frac{\delta}{\delta\chi(t')}\mathcal{S}[\chi]\right) = 0 \quad for\ t > t'$$

using the infinitesimal functions $\delta\chi$ and $\delta\chi'$ to define functional derivatives (as in subsection IIIA1 for the action).

In general, it is not possible to solve the Schrödinger equation for the propagator or the S-matrix exactly. One approximation scheme is the perturbation expansion in orders of the interaction:

$$H = H_0 + V \quad \Rightarrow \quad \mathcal{T}(e^{-i\int dt\ H}) = e^{-i(t_f - t_i)H_0} + \int_{t_i}^{t_f} dt\ e^{-i(t_f-t)H_0}[-iV(t)]e^{-i(t-t_i)H_0}$$
$$+ \int_{t_i}^{t_f} dt \int_{t_i}^{t} dt'\ e^{-i(t_f-t)H_0}[-iV(t)]e^{-i(t-t')H_0}[-iV(t')]e^{-i(t'-t_i)H_0} + \ldots$$

$$\Rightarrow \quad \mathcal{S}_{fi} \equiv \langle f|\mathcal{S}|i\rangle = \langle f|i\rangle + \int_{-\infty}^{\infty} dt\ \langle f,t|[-iV(t)]|i,t\rangle + \int_{-\infty}^{\infty} dt \int_{-\infty}^{t} dt'\ \langle f,t|[-iV(t)]e^{-i(t-t')H_0}[-iV(t')]|i,t'\rangle + ...$$

The first term in $\mathcal{S}$ is just the identity (i.e., the free piece). All the other terms consist of a string of interactions ($-iV$) connected by free propagators (e^{-itH_0}, where t is the time between the interactions), with each interaction integrated over all time (subject to time-ordering of the interactions), and the initial/final state (wave function) evaluated at the initial/final interaction time.

Exercise VA4.1

Assume the initial and final states are eigenstates of the free Hamiltonian:

$$H_0|i\rangle = E_i|i\rangle, \qquad H_0|f\rangle = E_f|f\rangle$$

Assuming V has no explicit time dependence, explicitly evaluate the time integrals in the S-matrix, effectively Fourier transforming from time to energy, to find

$$\mathcal{S}_{fi} = \langle f|i\rangle - 2\pi i\delta(E_f - E_i)\langle f|(E - H_0)\frac{1}{E - H + i\epsilon}(E - H_0)|i\rangle|_{E=E_i}$$

(Hints: Redefine the integration variables to be the times between interactions. Taylor expand $1/(E - H + i\epsilon)$ in V for comparison.)

In field theory we want to express any state in terms of a basis of products of 1-particle states, so we can calculate the behavior of these specified particles. We try to do this by using field variables (the "q's" of field theory): Each field operator should produce a single particle. Unfortunately, this is not the case: An asymptotic state of given 3-momentum created by such a field operator is not necessarily an eigenstate of the energy, because such a state can be either 1-particle or n-particle, due to interactions. The propagator for the field is then of the form

$$\hat{G}(p,t;p',t') \sim \delta(p - p') \sum_I \psi^*{}_I(p)\psi_I(p)e^{-i(t-t')E_I(p)}$$

$$E_I(p) = \sum_{i=1}^{n_I} E_{I,i}(p_i), \qquad \sum_{i=1}^{n_I} p_i = p$$

where "$E_{I,i}(p_i)$" is the energy of a 1-particle state (the $\sum_I$ will include an integral in general). However, as long as all particles have masses, such an asymptotic 1-particle state is distinguishable as that of lowest energy E_0: The higher-energy states are n-particle states to which this particle can couple. (If some of the n-particle states

were lower energy, the 1-particle state could decay into them, and thus the 1-particle state would be unstable, and not asymptotic. With massless particles things are more complicated: Then 1-particle states are more difficult to define and to measure.) In principle, we could define the 1-particle states by constructing the corresponding operator, consisting of the field plus terms higher order in the fields; in practice, this is rather complicated.

A simpler way to make the asymptotic states unambiguous is by modifying the definition of the S-matrix:

$$\mathcal{S} = \lim_{\substack{t_i \to -\infty(1+i\epsilon) \\ t_f \to +\infty(1+i\epsilon)}} e^{it_f H_0} \mathcal{T} \left(e^{-i \int_{t_i}^{t_f} dt\ H} \right) e^{-it_i H_0}$$

introducing factors of $1 + i\epsilon$ for some positive ϵ, which may be chosen small for convenience. (Actually, we can generally replace $1 + i\epsilon$ with just i if it is not too confusing: The result is the same.) The effect is seen by considering a matrix element of particular fields that may be a superposition of different energies E in the initial state and E' in the final state, but evaluated between an initial state of energy E_i and a final state of energy E_f (which might not be equal for a time-dependent interaction, e.g., if the number of particles changes). Since $E \geq E_i$ initially and $E' \geq E_f$ finally, the time dependence of any such matrix element is proportional to

$$\mathcal{S}_{fi} \sim \lim_{t_f \to +\infty(1+i\epsilon)} e^{it_f(E'-E_f)} \lim_{t_i \to -\infty(1+i\epsilon)} e^{-it_i(E-E_i)} = \begin{cases} 1 & for\ E = E_i, E' = E_f \\ 0 & otherwise \end{cases}$$

Alternatively, we can simply impose $E = E_i, E' = E_f$ directly in the definition:

$$\mathcal{S} = \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} e^{it_f H_0} \delta_{H(t_f),H_0} \mathcal{T} \left(e^{-i \int_{t_i}^{t_f} dt\ H(t)} \right) \delta_{H(t_i),H_0} e^{-it_i H_0}$$

where the free Schrödinger equation $H_0 = E_i$ or E_f defines E_i for the initial state and E_f for the final state, and δ_{H,H_0} is evaluated by examining the asymptotic time-dependence of the time-development operator with respect to t_i and t_f: Normally field theory is calculated in energy-momentum space, working with the spacetime Fourier transform of the above, where this amounts to simply comparing energies $E = E_i, E' = E_f$.

If we know some details of the interaction, this modification may be irrelevant: In particular, in local quantum field theory interactions happen at a point in space and time. For example, consider the inner product between a 1-particle state in its rest frame and a related n-particle state, which appears in the same propagator. Because of locality, the wave function for the n-particle state, when evaluated in position space

(which is where the theory is local) is simply the product of n 1-particle wave functions evaluated at the same point. But we know that for small relative momenta (where a nonrelativistic approximation holds) that the individual wave functions propagate as

$$|\psi| \sim |t - t'|^{-(D-1)/2}$$

from the form of the free 1-particle propagator. (Or, we can use dimensional analysis, and consider the spread of a particle of restricted range of momenta from a confined region: Then $|\psi|^2 \sim 1/V$ and the volume $V \sim |t - t'|^{D-1}$.) This implies that the n-particle wave function will fall off as the nth power of that, so in the limit of large times the 1-particle state will dominate. In a relativistic theory the length scale associated with this fall-off will be associated with the masses involved, and thus at a subatomic scale.

5. Wick rotation

In the previous subsection we ensured convergence in the definition of the S-matrix by effectively making the "coordinate change"

$$t \to (1 - i\epsilon)t = e^{-i\epsilon}t$$

in the definition of the limit

$$(1 - i\epsilon)t \to \infty \quad \Rightarrow \quad t \to (1 + i\epsilon)\infty$$

This affected the time-development operator as

$$e^{-iHt} \to e^{-iHt - \epsilon t}$$

for $H > 0$ to pick out the ground state $H = 0$. The same effective substitution was made in subsection VA3 in defining the contour integral for the propagator:

$$\int \frac{dE}{2\pi} e^{-iE(1-i\epsilon)t} \frac{i}{E - H} = \int \frac{dE}{2\pi} e^{-iEt} \frac{i}{(1 + i\epsilon)E - H}$$

$$= \int \frac{dE}{2\pi} e^{-iEt} \frac{i}{E - (1 - i\epsilon)H} = \int \frac{dE}{2\pi} e^{-iEt} \frac{i}{E - H + i\epsilon}$$

which is the same as the substitution

$$E \to (1 + i\epsilon)E = e^{i\epsilon}E$$

(when working with the time-independent Schrödinger equation) since essentially $E = i\partial/\partial t$.

In general, having to do contour integrals and keep track of $i\epsilon$'s in propagators is inconvenient. Fortunately, there is a simple way in practical calculations to get rid of not only the $i\epsilon$'s but (almost) all the other i's as well. The method is known as "Wick rotation". The basic idea is to extend the above complex rotation from angle ϵ to angle $\pi/2$:

$$t \to -it = e^{-i\pi/2}t, \qquad E \to iE$$

pushing the contour even farther away from the singularities. Thus, the Schrödinger equation is changed to a "diffusion equation" (to describe, e.g., Brownian motion):

$$(i\partial_t - H)\psi = 0 \quad \Rightarrow \quad (\partial_t + H)\psi = 0$$

For example, for the free particle the resulting equation has no i's. The time-independent Schrödinger equation then becomes

$$(E - H)\psi = 0 \quad \Rightarrow \quad (iE - H)\psi = 0$$

The result for the propagator is then

$$\int_{-\infty}^{\infty} \frac{dE}{2\pi}\, e^{-iEt} \frac{1}{H - iE} = \theta(t) e^{-Ht}$$

Now no $i\epsilon$ prescription is needed, since the pole was moved away from the real axis. Similar remarks apply to the inverse Fourier transform

$$\int_{-\infty}^{\infty} dt\; e^{iEt}\theta(t)e^{-Ht} = \frac{1}{H - iE}$$

Exercise VA5.1

Find the Wick-rotated retarded propagator $G(x', t'; x, t)$ for the free (1D) particle, satisfying

$$(\partial_t + H)G = (-\partial_{t'} + H')G = \sqrt{2\pi}\delta(x - x')\delta(t - t')$$

Furthermore, if we define the S-matrix directly in this Wick-rotated space

$$\mathcal{S} = \lim_{\substack{t_i \to -\infty \\ t_f \to +\infty}} e^{t_f H_0}\, \mathcal{T}\left(e^{-\int_{t_i}^{t_f} dt\; H}\right) e^{-t_i H_0}$$

then the limiting procedure is unambiguous even in field theory, since

$$\lim_{t_i \to -\infty} e^{t_i(E - E_i)} = \begin{cases} 1 & for\ E = E_i \\ 0 & for\ E > E_i \end{cases}$$

$$\lim_{t_f \to +\infty} e^{-t_f(E - E_f)} = \begin{cases} 1 & for\ E = E_f \\ 0 & for\ E > E_f \end{cases}$$