QFT-I: A conceptual summary

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What made quantum field theory necessary?

- Relativistic quantum mechanics has no way of dealing with the transmutation of particles.
- Relativistic quantum mechanics leads to negative probabilities & energy solutions.
- Relativistic quantum mechanics violates causality.

A relativistic Schrödinger equation

We start with the non-relativistic energy-momentum relation $\frac{p^2}{2m} = E$. First quantization of this (mapping the energy to the Hamiltonian operator and the momentum to its corresponding operator) yields the non-relativistic Schrödinger equation.

Scalars: Spin 0 particles (Bosons)

Preliminaries

If, instead, we start off by using the square of the *relativistic* energy-momentum relation and quantize this, we get the first version of the relativized Schrödinger equation: the Klein-Gordon equation.

$$(\Box + m^2)\phi(x) = 0$$

There are two main problems with this equation.

- Negative energy states: The energy eigenvalues satisfy $E = \pm\sqrt{p^2 + m^2}$. The negative energy solutions come from an extra term in the solution $\phi(x)$, which is present in this case only because we squared the original equation. A quick way to derive this is by using the fact that $e^{-ip_\mu x^\mu}$ is a solution.
- Negative probability densities: Using the same prescription of non-relativistic quantum mechanics to derive a probability density gives us an expression which is not positive-definite, thereby witholding us from interpreting it as a probability density. Once again, this is associated with the extra term in the solution of the equation.

These problems can be solved by reinterpreting $\phi(x)$ as a *quantum field* (which is an *operator*), rather than a wavefunction. But before understanding how, we must now perform second quantization in order to concretize this re-interpretation.

Borrowing from classical field theory, it is easily verifiable that the Lagrangian $\mathcal{L} = \frac{1}{2}(\partial^\mu\phi)(\partial_\mu\phi) - \frac{1}{2}m^2\phi^2$ will give rise to the Klein-Gordon equation (through the Euler-Lagrange equation). We now replace the Poisson bracket relation between ϕ and the canonical momentum, π, with a commutation relation (since both are now seen as operators).

An immediate question may be what these operators act on. The eigenstates of the Hamiltonian are now elements of a vector space known as *Fock space*, which is an algebraic extension of a Hilbert space. It is these elements that they act on.

We will compute the spectrum of the Klein-Gordon Hamiltonian in the next section and see that we no longer get any negative energy states.

The probability density is now an operator rather than a real-valued function. Its expectation value will give us the probability density, and since it is Hermitian (by construction), we will now no longer have any negative values for the same.

Catastrophe

We claimed two more advantages to quantum *field* theory over the framework of relativistic quantum mechanics: A story for the transmutation of particles, and a respect for causality. But first, let us deal with another problem our fresh paradigm has given us.

Using a Fourier mode decomposition based on the simple harmonic oscillator and using the classical field theoretic expression for the Hamiltonian, we get the following expression:

$$H = \int \frac{d^3k}{(2\pi)^3}\omega_k(a_k^\dagger a_k + \frac{1}{2}[a_k, a_k^\dagger])$$

Now, let $|0\rangle$ be the ground state; that is, it vanishes when acted on by a_k. Then, the energy of this ground state turns out to be $\sim \int d^3k\omega_k$, an integral which diverges! This 'infinite vacuum/zero-point energy' is a major unsolved problem in quantum field theory.

On the bright side, we get nice, finite eigenvalues when it acts on 'raised' energy eigenstates (that is, $|0\rangle$ acted upon by creation operators)—provided we pretend as if the vacuum energy term is zero.

Causality

Let us turn to the question of causality next.

Here was the problem: The amplitude for a free particle to propogate from x_0 to x was given by $\langle x|e^{-iHt}|x_0\rangle$. Using $H = \frac{p^2}{2m}$ and the identity resolution on $|p\rangle$, this can be computed to be $(\frac{m}{2\pi it})^{\frac{3}{2}} e^{im\frac{(x-x_0)^2}{2t}}$. Increasing the difference between the two points, the fact that this is nonzero for all t indicates a violation of causality. The situation is not helped with the obvious remedy of using the relativistic $E = \sqrt{p^2 + m^2}$ either.

Do things improve in the QFT framework? The propagator is the following:

$$D(x-y) = \langle 0|\phi(x)\phi(y)|0\rangle = \int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_p}e^{-ip\cdot(x-y)}$$

In the case $x-y$ is purely spatial, we have an expression which is exponentially vanishing but nonzero. However, some interpretative legwork will allow us to reconcile this with causality.

We must invoke a familiar principle from quantum mechanics: If two operators commute, their measurements cannot affect one another. What needs to be done in order to maintain causality is ensure that *information does not leak outside the light cone*; or, in our case, that the commutator of two fields vanishes for spacelike separations.

And the short answer is that, for a Klein-Gordon field, it does.

Transmutation

The third advantage of QFT had been that it offered an explanatory framework for the transmutation of elementary particles. Let us now delve into this through the example of meson decay.

A meson (created by the real scalar field ϕ) decays into a nucleon-antinucleon pair (created by the complex scalar field ψ). The process can be denoted mathematically by $|i\rangle \to |f\rangle$, where $|i\rangle = \sqrt{2E_p}a_p^\dagger|0\rangle, |f\rangle = \sqrt{4E_{q1}E_{q2}}b_{q1}^\dagger c_{q2}^\dagger|0\rangle$.

In principle, the amplitude for this can be computed by $\langle f|U|i\rangle$, the familiar quantum mechanical framework. (In practice, the time-evolution operator is, for a given Hamiltonian, given a perturbative expansion through the Dyson series. This thing is called the scattering matrix, and we usually ignore the higher-order terms in it. Wick's theorem is a helpful computational result.)

Spinors: Spin $\frac{1}{2}$ particles (Fermions)

Preliminaries

Another way to circumvent the problems enumerated above (negative energy states, negative probability densities) would be to try and end up with a *first*-order differential equation in time. Now, we had a second-order equation in the first place because we had started off with the *square* of the relativistic energy-momentum relation.

Therefore, historically, what Dirac did was cleverly take a square root of the wave operator p^2 and plug it back into the original Schrödinger equation.

Dirac tried taking the square root thus:

$$\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} = (A\partial_x + B\partial_y + C\partial_z + \frac{i}{c}D\partial_t)(A\partial_x + B\partial_y + C\partial_z + \frac{i}{c}D\partial_t)$$

Comparing the two sides reveals that the coefficients must be matrices, and yields the second version of the relativized Schrödinger equation: the Dirac equation.

$$(i\not{\partial} - m)\psi = 0$$

Notationally, $\not{\partial} = \gamma^\mu \partial_u$. Since γ^μ is a 4×4 matrix for each $\mu = 0, 1, 2, 3$, note that $\psi(x)$ must be a 4×1 matrix for this equation to make any sense. Each component $\psi_i(x)$ will satisfy the Klein-Gordon equation, as we will see.
This equation can be generated by the following Lagrangian:

$$\mathscr{L} = \bar{\psi}(i\not{\partial} - m)\psi$$

where $\bar{\psi} = \psi^\dagger\gamma^0$.

However, quantizing this equation in the previous manner gives rise to problems of its own.

Fermionic quantization

Recall that in the case of the Klein-Gordon equation, we used the operator to write an expression for the Hamiltonian; subsequently, we computed the eigenstates of the Hamiltonian (using a Fourier mode decomposition) and baptized them as the 'particles' of the field. Here, from the Lagrangian written above, we will have:

$$\mathscr{H} = \int d^3x \bar{\psi}(-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + m)\psi$$

What we want to do is find the spectrum of this Hamiltonian. This can be done through the following recipe:

- Find the plane-wave solutions of the Dirac equation.
- Write out the general form of the Dirac equation's solution.

This will be:

$$\psi(x) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2E_p}} e^{ip\cdot x} \sum_{s=1,2} (a_p^s u^s(p) + b_{-p}^s v^s(-p))$$

- Impose the canonical commutation relations and rewrite the Hamiltonian in terms of a, b.

This will give us:

$$\mathscr{H} = \int \frac{d^3p}{(2\pi)^3} \sum_s (E_p a_p^{s\dagger} a_p^s - E_p b_p^{s\dagger} b_p^s)$$

One can tell by computing the commutation relations between $\mathscr{H}$ and a, b that $a_p^{s\dagger}, b_p^{s\dagger}$ are positive energy particle (antiparticle resp.) creation operators; the other two are the destruction operators.

However, there is a serious problem: The eigenvalues of the particles created by $b_p^{s\dagger}$ operator are negative. First of all, this seems to mean that we can lower energy indefinitely.

Another point of discomfort arises when we compute the commutator $[\psi_a(x), \bar{\psi}_b(y)]$ to check the causality of this theory. We had skimmed over the details of this for the Klein-Gordon equation, but the upshot of it is the following: The propogation of a particle going one way outside the light cone was cancelled out by a term representing the propogation of an antiparticle going the opposite way. Here, however, the cancellation is between positive-energy and negative-energy particles propogating in the same direction.

It is positing *anticommutation* relations for the Dirac field which solves the negative energy problem; if, after doing this, we now simply redefine $b^\dagger \leftrightarrow b$, then all excitations will have positive energy. The fact that anticommutation relations are what work is closely related to the spin-statistics theorem; but we will not get into that for the time being.

Quantum Field Theory

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Autumn 2023

Path integrals in quantum mechanics

Discussion. The essential object we wish to compute with this formalism is the *propagator*: In other words, the probability for a particle to travel from one position to another in a given amount of time.
Let our initial coordinates be (x, t_i), and the final coordinates be $(x_f, t_f); t_f > t_i$. We know that the Schrödinger equation is linear. This makes it possible for us to write the following expression:

$$\psi(x_f, t_f) = \int_{-\infty}^{\infty} K(x_f, t_f, x, t_i)\psi(x, t_i)dx$$

(In a crude sense, this equation expresses the expansion of a vector in terms of a basis.)
Now, the quantity $K(x_f, t_f, x, t_i)$ is called the propagator. There is an alternative characterization of it: If we have something which satisfies the following 'modified' Schrödinger equation:

$$(i\hbar\frac{\partial}{\partial t} - H)K(x_f, t_f, x, t) = i\hbar\delta(x_f - x)\delta(t_f - t)$$

and the following boundary condition:

$$lim_{\epsilon\to 0^+} K(x, t_f + \epsilon, x, t) = i\hbar\delta(x_f - x)$$

then we've found the propagator. (This tells us that the propagator is a Green's function for the Schrödinger equation.)

Discussion. We will now derive an explicit formula for the propagator. Let $\varphi_n(x)$ be the energy eigenfunctions, and let $\psi(x, t_i) = \sum a_n\varphi_n(x)$. Then, we know that

$$\psi(x, t) = \sum a_n e^{-iE_n\frac{(t-t_i)}{\hbar}}\varphi_n(x) = \sum(\int \varphi_n^*(x')\psi(x', t_i))e^{-iE_n\frac{(t-t_i)}{\hbar}}\varphi_n(x)$$

After some simplification and the insertion of the Θ operator to ensure causality is respected, we have the following:

$$K(x, t, x', t_i) = \Theta(t - t_i)\sum_n \varphi_n(x)\varphi_n^*(x')e^{-iE_n\frac{(t-t_i)}{\hbar}}$$

There's a more suggestive way to write out the above formula. Using the fact that $\varphi_n(x) = \langle x|\varphi_n\rangle$ and the identity theorem $\sum|\varphi_n\rangle\langle\varphi_n| = I$, we get

$$K(x, t, x', t_i) = \langle x|e^{-iH\frac{(t-t_i)}{\hbar}}|x'\rangle = \langle x|e^{-iH\frac{(t-t_0)}{\hbar}}e^{iH\frac{(t_i-t_0)}{\hbar}}|x'\rangle = \langle x, t|x', t_i\rangle,$$

which is *exactly* the inner product one would think of, quantum mechanically, when speaking of the probability $x', t_i \mapsto x, t$.

Example. Let's compute a small example: The case of the free particle propagator.
We start with the Fourier transform formula:

$$\psi(x,t_i) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\varphi(p)e^{\frac{ipx}{\hbar}}dp$$

and

$$\varphi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x,t_i)e^{\frac{ipx}{\hbar}}dx$$

Now,

$$\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\varphi(p)e^{\frac{ipx}{\hbar}}e^{-i\frac{p^2(t-t_i)}{2m\hbar}}dp$$

Plugging the second equation into the third, it becomes possible to read off the result:

$$K(x,t,x',t_i) = \frac{1}{2\pi\hbar}\int_{\infty}^{\infty}\exp[\frac{-i(t-t_i)p^2}{2m\hbar} + \frac{i(x-x')p}{\hbar}]dp$$

This is a Gaussian integral. Upon evaluation, we get:

$$\sqrt{\frac{m}{i2\pi\hbar(t-t_i)}}\exp(-\frac{i}{2\hbar}\frac{m(x-x')^2}{(t-t_i)})$$

Note that the expression in the exponent is, in the limit, nothing but the classical action (modulo the factor).

Discussion. Let's return to the formulation we had arrived at last:
$K(x_f,t_f,x_i,t_i) = \langle x_f,t_f|x_i,t_i\rangle\Theta(t_f-t_i)$. Once again using the identity resolution on $|x,t\rangle$, we get, for $t_i < t < t_f$ (so that we can use the factorization property on Θ),

$$K(x_f,t_f,x_i,t_i) = \int_{-\infty}^{\infty}K(x_f,t_f,x,t)K(x,t,x_i,t_i)dx$$

What we're actually doing here is summing over all the possible routes it could take, wherein each route is characterized by where it is at the time t. Iterating this lends an easy generalization:

$$K(f|0) = \int(\Pi_{i=1}^{n}(K(i|i-1)dx_i))K(f|n)$$

Conceptually, we're still doing the same thing; only that a given possible route is now characterized by the positions at n many time slices, so that the total probability of following it is (familiarly enough) given by the relevant product.
Naturally, we want to generalize this to a continuum—infinitely many—of these so-called 'time-slices'. What this would amount to is $\max(t_{i+1}-t_i)\to 0$. Consider, then, the following approximation, which works in our limit:

$$e^{-\frac{i\epsilon}{\hbar}H} = 1 - \frac{i\epsilon}{\hbar}(\frac{p^2}{2m}+V(x)) + O(\epsilon^2) = (1-\frac{i\epsilon}{\hbar}\frac{p^2}{2m})(1-\frac{i\epsilon}{\hbar}V(x)) + O(\epsilon^2) \sim e^{(-\frac{i\epsilon}{\hbar}\frac{p^2}{2m})}e^{(-\frac{i\epsilon}{\hbar}V(x))}$$

So,

$$K(i+1|i) = \int_{-\infty}^{\infty}dp_i e^{(-\frac{i\epsilon}{\hbar}\frac{p^2}{2m})}e^{(-\frac{i\epsilon}{\hbar}V(x_i))}\langle x_{i+1}|p_i\rangle\langle p_i|x_i\rangle$$

Using the fact that $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{ixp}{\hbar}}$ and evaluating the integral, we'll get:

$$K(i+1|i) = \sqrt{\frac{m}{i\epsilon 2\pi\hbar}}e^{\frac{i}{\hbar}\epsilon(\frac{m}{2}\frac{(x_{i+1}-x_i)^2}{\epsilon^2}-V(x_i))}$$

Discussion. Let's put everything together now. Recall that $K(n+1|0) = \int(\Pi_{i=0}^{n} K(i+1|i))(\Pi_{i=1}^{n} dx_i)$. Plugging in what we computed previously and taking the limit $n \to 0$,

$$\begin{aligned} K(final|initial) &= \int \lim_{n\to\infty}(\Pi_{i=1}^{n} dx_i)\left(\frac{m}{i\epsilon 2\pi\hbar}\right)^{\frac{n+1}{2}} e^{[\frac{i\epsilon}{\hbar}\sum_{j=0}^{n}[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 - V(x_j)]]} \\ &= \int \mathscr{D}_x \exp[\frac{i}{\hbar}\int_{t_i}^{t_f} dt\mathscr{L}(x,\dot{x})] \\ &= \int \mathscr{D}_x \exp[\frac{i}{\hbar}S_{i\to f}] \end{aligned}$$

where $\mathscr{D}_x = \lim_{n\to\infty}(\Pi_{i=1}^{n} dx_i)(\frac{m}{i\epsilon 2\pi\hbar})^{\frac{n+1}{2}}$.

Mathematical interlude: Gaussian integrals

Lemma 1.1. $\int_{-\infty}^{\infty} e^{-ax^2+bx+c}dx = \sqrt{\frac{\pi}{a}}e^{\frac{b^2}{4a}+c}$, *assuming Re(a)>0.*

The proof merely involves factorization and substituting variables appropriately.

Lemma 1.2 (Multivariate Gaussian integral)**.** *Let A be an $n \times n$ matrix with constant entries, b, c be an $n \times 1$ matrix with constant entries and X be an $n \times 1$ matrix with the variable entries. Then,* $\int_{-\infty}^{\infty} dx_1...dx_n e^{X^TAX+b^TX+C} = \frac{\pi^{\frac{n}{2}}}{\sqrt{DetA}}e^{\frac{1}{4}b^tA^{-1}b+C}$

Example. It will now be instructive to compute the free particle propagator using the more general path integral formalism.
In this case, the potential $V = 0$. So $K_n = \int(\Pi_{i=1}^{n} dx_i)(\frac{\alpha}{\pi})^{\frac{n+1}{2}} e[-\alpha\sum_{i=0}^{n}(x_{i+1}-x_i)^2]$, where $\alpha = \frac{m}{i2\epsilon\hbar}$.
$K_n = (\frac{\alpha}{\pi})^{\frac{n+1}{2}} e^{-\alpha(x_{n+1}^2+x_0^2)}\int(\Pi_{i=1}^{n} dx_i)e^{2\alpha(x_1x_0+x_nx_{n+1})}e^{-2\alpha(x_1^2+...+x_n^2-x_1x_2-...-x_{n-1}x_n)}$.

Now, set $X = \begin{pmatrix} x_1 \\ . \\ . \\ . \\ x_n \end{pmatrix}, b = 2\alpha \begin{pmatrix} x_0 \\ 0 \\ . \\ 0 \\ x_{n+1} \end{pmatrix}, A = \begin{pmatrix} 2 & -1 & 0 & ... & ... & 0 \\ -1 & 2 & -1 & 0 & ... & 0 \\ 0 & -1 & 2 & -1 & ... & 0 \\ . & & & & & \\ . & & & & & \\ . & & & & & \\ 0 & ... & ... & 0 & -1 & 2 \end{pmatrix}$

Then, we have $K_n = (\frac{\alpha}{\pi})^{\frac{n+1}{2}} e^{-\alpha(x_{n+1}^2+x_0^2)}\int(\Pi_{i=1}^{n} dx_i)e^{X^TAX+b^TX}$.
One can compute that $\mathrm{Det}A = \alpha^n(n+1)$.
Then, using the above lemma, we have $K_n = \sqrt{\frac{\alpha}{\pi(n+1)}}e^{-\frac{\alpha}{n+1}(x_{n+1}-x_0)^2}$.
To get the final expression, we need to take the limit $n \to \infty$ in the above. Doing so, we get:

$$K(F|I) = \sqrt{\frac{m}{i2\pi\hbar(t_f-t_i)}}\exp(-\frac{i}{2\hbar}\frac{m(x_f-x_i)^2}{(t_f-t_i)})$$

which is exactly what we had with the first method.

Example. A remark may be made on how the path integral formalism reproduces, in the limit, the classical principle of stationary action.
We are concerned with integrals of the following form:

$$\int_{-\infty}^{\infty} dx e^{\frac{i}{\hbar} f(x)}$$

The *stationary phase approximation* states that as the ratio $\frac{f(x)}{\hbar}$ becomes vanishingly small, the integral over any interval will be vanishingly small—unless one is near a critical point of $f(x)$.
In the classical limit, the ratio of $\frac{S}{\hbar}$ will indeed become vanishingly small as S increases; and as per the approximation, the contribution to the integral will come precisely from that path which is a critical point for S; this, of course, is nothing but the principle of least action.

Discussion. We can generalize this to quantum systems described by Hamiltonians over a general phase space, $H(q,p)$.
We want to compute the transition amplitude $U(q_a, q_b; T) = \langle q_b | e^{-iHT} | q_a \rangle$ (setting $\hbar = 1$ for convenience). Once again, we will be introducing a set of intermediate states and breaking the exponential into short slices.
This will leave us with a product of factors of the form $\langle q_{k+1} | e^{-iH\epsilon} | q_k \rangle \sim \langle q_{k+1} | 1 - iH\epsilon + ... | q_k \rangle$.
Now, we claim that, for a Hamiltonian which contains products of p, q in the right order (this is known as a *Weyl ordered* Hamiltonian), the following holds:

$$\langle q_{k+1} | H(p,q) | q_k \rangle = (\Pi_i \int \frac{dp_k^i}{2\pi}) H(\frac{q_{k+1} + q_k}{2}, p_k) \exp[i \sum_i p_k^i (q_{k+1}^i - q_k^i)]$$

This is not too hard to derive. The Fourier transform of the Dirac delta function is used an an intermediary step. So, we finally get

$$\langle q_{k+1} | e^{-i\epsilon H} | q_k \rangle = (\Pi_i \int \frac{dp_k^i}{2\pi}) \exp(-i\epsilon H(\frac{q_{k+1} + q_k}{2}, p_k)) \times \exp(i \sum_i p_k^i (q_{k+1}^i - q_k))$$

There were N factors like this which we multiply together (and integrate over q) to get the final expression:

$$U(q_a, q_b; T) = (\Pi_{i,k} \int dq_k^i \int \frac{dp_k^i}{2\pi}) \exp(i \sum_k (\sum_i p_k^i (q_{k+1}^i - q_k) - \epsilon H(\frac{q_{k+1} + q_k}{2}, p_k))$$

which is nothing but the discretized form of

$$U(q_a, q_b; T) = (\Pi_i \int \mathcal{D}(q,p)) \exp(i \int_0^T dt (\sum_i p^i \dot{q}^i - H(q,p)))$$

Path integrals in quantum field theory

Scalar fields

The following is the apparent analogue of the path integral for field theories:

$$\int \mathscr{D}[\phi]\exp(i\int_0^T d^4x\mathscr{L})$$

where $\mathscr{L} = \frac{1}{2}(\partial_\mu\phi)^2 - V(\phi)$.
This is an integral over *all possible field configurations in spacetime.* In order to make sense of this, we must perform a process known as **regularization**.

Discussion. Regularization comes in two flavours. Suppose we are working in $d-$dimensional Minkowski space.

1. Ultraviolet regularization: We pretend as if space-time is discrete at small scales.
   First, send $\mathscr{D}[\phi] \to \Pi_{I\in\mathbb{Z}^d} d\phi(I)(\frac{2i\pi\hbar}{\epsilon^{d-2}})$, where ϵ is the space-time 'cutoff'; that is, we only have (x,t) of the form $(i\epsilon, j\epsilon)$ for $(i,j) \in \mathbb{Z}^d$.
   Next, we must discretise the action. This yields

   $$S[\phi] = \sum_{I\in\mathbb{Z}^d} \epsilon^d \frac{1}{2}m^2((\frac{\phi(I+e_0)-\phi(I)}{\epsilon})^2 - \sum_{a=1}^{d}(\frac{\phi(I+e_a)-\phi(I)}{\epsilon})^2 - \phi(I)^2)$$

   (where the terms are so-called finite difference derivatives.)
   We will ultimately let $\epsilon \to 0$ to recover the original limit.

2. Infrared regularization: In this case, we impose periodicity conditions on space-time (so, our ambient space becomes a higher-dimensional torus) and later let the periods tend to infinity.

Remark. Where does the mysterious factor in ultraviolet regularization come from?

Definition (Functional derivatives)**.** *Let $J[y]$ be a functional with differential $\delta J[h]$ at $h(x)$, where $f(x) = y$. Then, the **functional derivative** of J at h with respect to f is the function $\frac{\delta J}{\delta y}$ such that $\delta J[h] = \int \frac{\delta J}{\delta y}(x)h(x)dx$*

Remark. In computations, one often uses the formula $\frac{\delta F(f(x))}{\delta f(y)}(x) = lim_{\epsilon\to 0}\frac{F(f(x)+\epsilon\delta(x-y))-F(f(x))}{\epsilon}$. However, this equivocation is not quite rigorous.

Lemma 2.1. *The functional derivative satisfies the following properties:*

1. *Linearity, product rule & chain rule*
2. $\frac{\delta J(y)}{\delta J(x)} = \delta(x-y)$

Remark. We can make sense of the expression in 2 for any ordinary function as well by writing it as an integral via the Dirac delta.

Discussion. In canonical quantization, one evaluates the amplitude of any process by recasting it into a scattering matrix/unitary time-evolution operator and using Wick's theorem on the perturbative expansion. Finally, the Feynman rules are produced based on the terms we get after computation. The first step in this utilizes the Hamiltonian dynamics, which we have forgone with the path integral formalism. Let us work out the same procedure for a free scalar theory in this framework.

Discussion. This three-step calculation takes us from the correlation function to the propagator term (and thus, the Feynman diagram) for the simplest possible process. The detailed algebra for each step in the derivation can be found either in Peskin & Schroeder or Das.

- $\langle 0|T\phi(x_1)\phi(x_2)|0\rangle = \frac{\int \mathcal{D}\phi\phi(x_1)\phi(x_2)\exp[i\int d^4x\mathcal{L}]}{\int \mathcal{D}\phi\exp[i\int d^4x\mathcal{L}]}$
- $\frac{\int \mathcal{D}\phi\phi(x_1)\phi(x_2)\exp[i\int d^4x\mathcal{L}]}{\int \mathcal{D}\phi\exp[i\int d^4x\mathcal{L}]} = \frac{1}{Z_0}(-i\frac{\delta}{\delta J(x_1)})(-i\frac{\delta}{\delta J(x_2)})Z[J]|_{J=0}$
  where $Z[J] = \int \mathcal{D}\phi\exp[i\int d^4x[\mathcal{L} + J(x)\phi(x)]]$ (the *generating functional*) and $Z_0 = Z[J=0]$
- $\frac{1}{Z_0}(-i\frac{\delta}{\delta J(x_1)})(-i\frac{\delta}{\delta J(x_2)})Z[J]|_{J=0} = D_F(x_1 - x_2)$

Higher correlation functions can be computed simply by taking higher functional derivatives of the generating functional, and it can be checked that it produces exactly the same results as in canonical quantization.

Example. Let us now repeat the above exercise for an interacting scalar field; in particular, for ϕ^4 theory ($\mathcal{L} = \frac{1}{2}(\partial_\mu\phi) + \frac{m^2}{2}\phi^2 + \frac{g}{4!}\phi^4$).
First of all, note that we never computed the interacting field correlation functions in QFT—I. We were able to compute the scattering amplitudes directly using Wick's theorem (which, in turn, relied only on the free field correlation function).
The idea here, that we can know scattering matrix amplitudes if we compute the relevant field correlation functions, relies on the *LSZ reduction formula*, something we have yet to see. Nonetheless, let us compute the latter.

- $\langle\Omega|T\phi(z_1)\phi(z_2)...\phi(z_n)|\Omega\rangle = \frac{\int \mathcal{D}\phi\phi(z_1)\phi(z_2)...\phi(z_n)\exp[i\int d^4x\mathcal{L}]}{\int \mathcal{D}\phi\exp[i\int d^4x\mathcal{L}]}$: This formula still holds true, with derivation unchanged. (Note that Ω is the *interaction* vacuum, whereas $|0\rangle$ is the free field vacuum.)
- $\frac{1}{Z_0}\int \mathcal{D}\phi\phi(z_1)\phi(z_2)...\phi(z_n)\exp[i\int d^4x\mathcal{L}] =$
  $\sum_{k=0}^{\infty}\frac{1}{k!}(\frac{-g}{\hbar 4!})^k\int d^4x_1...d^4x_k\langle 0|T\phi(z_1)\phi(z_2)...\phi(z_n)\phi^4(x_1)...\phi^4(x_k)|0\rangle$: Multiply and divide by Z_0, expand the exponential, interchange the sum with the integral.

Note that the odd-point correlation functions will vanish (this can be checked by expanding them in terms of the creation/annihilation operators, etc.).
The third formula gives us a way to evaluate the numerator of the correlation function. One can read off the Feynman diagrams (using Wick's theorem) for a given $n-$point and order. There will be a number of vacuum bubbles. The nice thing is that these will *exactly* be cancelled out by the denominator:
$\frac{1}{Z_0}\int \mathcal{D}\phi\exp[i\int d^4x\mathcal{L}] = \sum_{k=0}^{\infty}\frac{1}{k!}(\frac{-g}{\hbar 4!})^k\int d^4x_1...d^4x_k\langle 0|T\phi^4(x_1)...\phi^4(x_k)|0\rangle$.

Interlude: LSZ Reduction

The idea of LSZ reduction is to obtain a formula for scattering processes (particles entering from $-\infty$, being subjected to something and exiting to $+\infty$) in terms of correlation functions. We begin with the following:

$$\langle\Omega|T\{\phi(z_1)...\phi(z_{n+2})\}|\Omega\rangle$$

The required formula will be obtained when we successfully Fourier transform this.
First, some setup:

- $|\Omega\rangle$: The interaction vacuum
- $\mathbf{P}$: The three-momentum operator
- $\mathbf{H}$: The Hamiltonian
- $|\lambda_p\rangle$: Eigenstates of the Hamiltonian with momentum p
- $E_p(\lambda)$: Energy of the eigenstate $\lambda_p\rangle$

The following identities will be used by us variously:

$$\mathbf{1} = |\Omega\rangle\langle\Omega| + \sum_{\lambda}\int \frac{d^3p}{(2\pi)^3}\frac{1}{2E_p(\lambda)}|\lambda_p\rangle\langle\lambda_p|$$

$$\langle\Omega|\phi(x)|\lambda_p\rangle = \langle\Omega|\phi(0)|\lambda_0\rangle e^{-ipx}|_{p^0=E_p}$$

The completeness relation appear a bit odd to look at to begin with, because of the mix of discrete and continuous sums. The continuous part sums over the three-momentum, while the discrete part sums over the 0th (energy) component. The first term is merely the zero-energy state, and the sum will run over all zero-momentum energy eigenstates $|\lambda_0\rangle$. While the identity operator will be inserted in the previous expression during calculations, we will ignore the first term because it will always be finite, *sans* singularities.

First, we describe how to simplify the transform against one argument, $\int d^4x e^{ipx}\langle\Omega|T\{\phi(x)...\phi(z_{n+2})\}|\Omega\rangle$:

- Divide the integral over x^0 into three regions: $-\infty$ to T^-, where $T^- < z_i^0$, T^- to T^+, T^+ to ∞, where $T^+ > z_i^0$. The second region will be analytic in p^0. Consider region III for the time being.
- Insert the identity operator (indexed by q) and use the second relation.
- Integrate over d^3x. This will yield a $\delta^3(p-q)$.
- Integrate over d^3q, after inserting a factor of $e^{-\epsilon x^0}$ to ensure everything is well-defined.

At this stage, we are left with the following expression:

$$\sum_{\lambda}\frac{1}{2E_p(\lambda)}\frac{ie^{(p^0-E_p(\lambda)+i\epsilon)}}{p^0-E_p(\lambda)+i\epsilon}\langle\Omega|\phi(0)|\lambda_0\rangle\langle\lambda_p|T\{\phi(z_2)...\phi(z_{n+2})\}|\Omega\rangle$$

Note that, near poles, $2E_p(\lambda) \sim p^0 + E_p(\lambda)$, so that in the denominator, we have $(p^0)^2 - E_p(\lambda)^2$. Our final result is as follows:

$$\int d^4x e^{ipx}\langle\Omega|T\{\phi(x)...\phi(z_{n+2})\}|\Omega\rangle \sim_{p^0\to E_p} \frac{i}{p^2-m^2+i\epsilon}\sqrt{Z}\langle\mathbf{p}|T\{\phi(z_2)...\phi(z_{n+2})\}|\Omega\rangle$$

where $Z = |\langle\Omega|\phi(0)|\lambda_0\rangle|^2$, the 'field strength renormalization factor'. In exactly the same manner, the integral in region I evaluates to:

$$\int d^4x e^{ipx}\langle\Omega|T\{\phi(x)...\phi(z_{n+2})\}|\Omega\rangle \sim_{p^0\to -E_p} \frac{i}{p^2-m^2+i\epsilon}\sqrt{Z}\langle\Omega|T\{\phi(z_2)...\phi(z_{n+2})\}|-\mathbf{p}\rangle$$

We now want to do this for all the fields in the time-ordering. For this, we will need to be able to make the approximation $|\lambda_{p_1}\lambda_{p_2}\rangle \sim |\lambda_{p_1}\rangle \otimes |\lambda_{p_2}\rangle$. This can be done by isolating each of them in position-space, i.e., diffusing them in momentum-space:

$$\int d^4x e^{ip^0x^0}e^{i\mathbf{px}} \to \int \frac{d^3k}{(2\pi)^3}\int d^4x e^{ip^0x^0}e^{-i\mathbf{kx}}\varphi(\mathbf{k})$$

where $\varphi(\mathbf{k})$ is a distribution centred at $\mathbf{p}$. The original expression will be multiplied by such a wavepacket for each of the $(n+2)$ fields. Now, we describe how to evaluate this (for, say, two fields having $x_i^0 > T^+$, the rest $< T^-$):

- Repeat the first step of the previous process.
- Insert the identity operator, indexed by K. Break it up into a product of $n+2$ integrals (and a sum with $n+2$ indices), using our wavepacket approximation.
- Use the second relation on each of the $n+2$ terms, and evaluate each of the $\int d^3q_i$. Consider the dominant terms near the poles (this is the first limit).
- Let the wavepackets tend to delta functions (this is the second limit).
- Repeat the above steps for the fields in the 'past'.

Finally, we have, as the maximally singular term:

$$(\prod_{i=1,2}\frac{i}{p_i^2-m^2+i\epsilon}\sqrt{Z})(\prod_{i=3,..,n+2}\frac{i}{p_i^2-m^2+i\epsilon}\sqrt{Z})\langle p_1p_2|S|-p_3...\rangle$$

(note that the states are of 3-momentum).

Theorem 2.2 (Lehmann-Symanzik-Zimmermann)**.** *The limit taken in order of pole first, delta function second is the same as taking the limit of the delta functions first, and at the poles second.*

This yields the LSZ reduction formula:

$$\prod_{i=1}^{n}\int d^4x_i e^{ip_ix_i}\prod_{j=1}^{m}\int d^4y_j e^{-ik_jy_j}\langle\Omega|T\{\phi(x_1)...\phi(x_n)\phi(y_1)...\phi(y_m)\}|\Omega\rangle\sim$$

$$(\prod_{i=1}^{n}\frac{i}{p_i^2-m^2+i\epsilon}\sqrt{Z})(\prod_{j=1}^{m}\frac{i}{p_j^2-m^2+i\epsilon}\sqrt{Z})\langle p_1...p_n|S|k_1...k_m\rangle$$