PTJC Talk #2: QFT → Lattice

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October 16, 2017

(1) QFT Path Integrals

Last week, Dake told us about path integrals in quantum mechanics and how to study them numerically by discretizing time. Results looked a lot like stat mech and we have good MCMC methods for doing this kind of problem. This week, we're going to do the same thing to quantum field theory, which turns out to be harder.

Overview:

- Path integrals in Minkowski continuum; why do we care?
- Wick rotation → Euclidean time
- Spacetime discretization
- Lattice calculations
- Going back? (Reflection positivity)

(real scalar fields throughout today)

In QFT we like to calculate time-ordered correlators of fields:

$$G(x_1, \ldots, x_n) = \langle 0| T\left[\hat{\phi}(x_1) \cdots \hat{\phi}(x_n)\right] |0\rangle \tag{1.1}$$

$$\phi(x_1) = e^{-ip\cdot x}\hat{\phi}(0)e^{+ip\cdot x} \tag{1.2}$$

LSZ tells us we can recover good things from these. A standard derivation lets us rewrite them as

$$G(x_1, \ldots, x_n) = \frac{\int[\mathcal{D}\phi]e^{iS}\phi(x_1)\cdots\phi(x_n)}{\int[\mathcal{D}\phi]e^{iS}} \quad (\phi(x_i) \text{ now just numbers}) \tag{1.3}$$

$$S = \int \mathrm{d}^4x \left[-\frac{(\partial_\mu\phi)(\partial^\mu\phi)}{2} - V(\phi)\right]. \tag{1.4}$$

But this is terrible! $\int[\mathcal{D}\phi]$ scares mathematicians, and it should scare us too! Even if we deal with that, the e^{iS} exponential is highly oscillatory.

As humans, we have some coping strategies for this situation ("sourceology", etc), but we want to find these things with a computer. Clearly we need to adapt this.

(a) Wick Rotation

First thing we can do is

$$x^0 \to -ix_4 \quad \text{(n.b. clockwise)}. \tag{1.5}$$

We will now write position vectors $x_E = (x_1, \ldots, x_4)$, metric is all 1s. What does this do? Well,

$$ip \cdot x = -iHt + i\vec{p} \cdot \vec{x} \to ip \cdot x_E = -Ht + i\vec{p} \cdot \vec{x}. \tag{1.6}$$

so look at the propagator

$$G(x, 0) = \langle 0| e^{-ip\cdot x} \hat{\phi}(0) e^{ip\cdot x} \hat{\phi}(0) |0\rangle \to G_E(x_E, 0) = \langle 0| \underbrace{e^{+Ht - i\vec{p}\cdot\vec{x}}}_{\to 0} \hat{\phi}(0) e^{-Ht + i\vec{p}\cdot\vec{x}} \hat{\phi}(0) |0\rangle \tag{1.7}$$

Manifest exponential suppression at large Euclidean times. Insert some complete sets of states, get

$$G_E(x_E, 0) = \sum_n |\langle 0| \hat{\phi}(0) |0\rangle|^2 e^{-E_n x_4} e^{i\vec{p}_n \cdot \vec{x}}, \tag{1.8}$$

so (assuming H bdd below) we have a unique ground state that dominates at big x_4, can extract energy from this if calculated.

This makes all of our correlators nicer, but they're still difficult to calculate, so we turn to the path integral. We can derive it just as well in Euclidean space, finding

$$G_E(x_1, \ldots, x_n) = \frac{\int [\mathcal{D}\phi] e^{-S_E} \phi(x_1) \cdots \phi(x_n)}{\int [\mathcal{D}\phi] e^{-S_E}}, \tag{1.9}$$

$$S_E = -iS = \int \mathrm{d}^4 x \left[+\frac{1}{2} (\partial_\mu \phi)(\partial_\mu \phi) + V(\phi) \right] \tag{1.10}$$

(n.b. that derivatives are on $\{x_1, x_2, x_3, x_4\}$ and up/down no longer matters)

The kinetic term is strictly positive, so highly oscillatory field configurations are damped and contribute less. This is encouraging for numerics.

Danger!

We took our Minkowski theory with Hamiltonian time evolution and rotated it to a Euclidean theory which we're about to put on the lattice. In practice, we're ultimately going to be defining a lattice action based on a Euclidean action as our starting point. Do we know how to go back? Can our Euclidean theory be analytically continued to a *physical* Minkowski theory? Or are we making garbage? The answer is "sometimes". Will talk later about conditions for going back.

(2) Latticization

Okay, so we've got a path integral expression for our Euclidean correlators, which seem easier to calculate. However, we've still got that pesky $[\mathcal{D}\phi]$ running around and meanwhile we've imposed no regularization at all. Let's kill two birds with one stone by putting everything on a lattice.

We'll choose a hypercubic lattice Λ: same spacing a in all four directions. Not mandatory, but convenient. Note that right away we are down to a finite subgroup of rotations, with a group of discrete translations depending on the size of the lattice.

$$x \to na \tag{2.1}$$

$$n = (n_1, n_2, n_3, n_4) \in \mathbb{Z}^4 \tag{2.2}$$

$$a\phi(x) \to \phi_n \tag{2.3}$$

$$\int \mathrm{d}^4 x \to a^4 \sum_n \tag{2.4}$$

We describe unit steps along coordinate directions on the lattice with vectors μ, used as an index.

These ones are pretty straightforward, but what to do about derivatives? If you've done basic numeric ODE solving you know there are several choices. We'd like something local and symmetric. A good choice for this will come by demanding not that the lattice kinetic term reduces directly to the ctm one, but that the *action* reduces to the ctm action. With this in mind we can integrate by parts the kinetic term

$$\int \mathrm{d}^4 x\, [(\partial_\mu \phi)(\partial_\mu \phi)] = -\int \mathrm{d}^4 x\, \phi \partial_\mu^2 \phi + \text{surface term.} \tag{2.5}$$

To make the surface term vanish, we must either assume we're on an infinite lattice *or* impose periodic boundary conditions in each direction on a finite lattice. In numerical practice we'll do the latter. The second derivative is now discretized in the way familiar from Verlet integration, giving

$$a^4 \phi \partial_\mu^2 \phi \to \sum_\mu \phi(\phi_{n+\mu} + \phi_{n-\mu} - 2\phi_n). \tag{2.6}$$

Our action is more polite now, but we haven't dealt with the functional measure. Fortunately, it's straight forward:

$$\int [\mathcal{D}\phi] \to \prod_n \int \mathrm{d}\phi_n. \tag{2.7}$$

Now everything is lovely!

$$S = \frac{1}{2} \sum_{n,\mu} -\phi_n \left(\phi_{n+\mu} + \phi_{n-\mu} - 2\phi_n\right) + \sum_n V(\phi_n) \tag{2.8}$$

$$Z = \prod_n \left[\int \mathrm{d}\phi_n \right] e^{-S} \tag{2.9}$$

$$G_N(n_1, \ldots, n_N) = \frac{\prod_n \left[\int \mathrm{d}\phi_n\right] e^{-S} \phi_1 \cdots \phi_N}{Z} \tag{2.10}$$

We've gone from an ill-defined, highly oscillatory integral to a real, likely convergent, countable or finite set of integrals.

Regularization

Note that in moving to the lattice we've imposed a momentum cutoff. Much as in crystal physics, momenta outside the first Brillouin zone are aliased to momenta within it, so each momentum component satisfies

$$k_\mu \in \left[-\frac{\pi}{a}, \frac{\pi}{a}\right]. \tag{2.11}$$

This means all of our momentum integrals are over a compact, bounded domain and makes our theory UV-finite.

(a) Continuum limits

We should be a little worried at this point. We've made a lot of choices in how to go from our Minkowski theory to a Euclidean theory to a lattice theory. Does it matter? Yes, definitely. There are infinitely many lattice actions corresponding to a given Euclidean ctm action. This is critical to, e.g., implementing fermions, but also means that it may not be obvious how to get back from the lattice. This will be important in later talks.

(b) Free propagator example

We now have enough technology to do a simple lattice example: the free propagator.

$$G(n,p) = \frac{1}{Z}\left[\prod_\ell \int \mathrm{d}\phi_\ell\right] e^{-S}\phi_n\phi_p \tag{2.12}$$

$$S = \sum_{n,\mu} -\frac{1}{2}\phi_n\left[\phi_{n+\mu}+\phi_{n-\mu}-2\phi_n\right] + \frac{1}{2}m^2\sum_n \phi_n \tag{2.13}$$

Note that $m = m^{\text{phys}}a$. Rewrite as quadratic form

$$S = \frac{1}{2}\phi_n M_{np}\phi_p \tag{2.14}$$

$$M_{np} = \delta_{np}\left(m^2+8\right) - \sum_\mu\left(\delta_{n,p+\mu}+\delta_{n,p-\mu}\right) \tag{2.15}$$

This is a multi-dimensional Gaussian integral and we'll get

$$Z = \frac{(\sqrt{2\pi})^{|\Lambda|}}{\sqrt{\det M}} \tag{2.16}$$

$$\left[\prod_\ell \mathrm{d}\phi_\ell\right] e^{-S}\phi_n\phi_p = \frac{(\sqrt{2\pi})^{|\Lambda|}}{\sqrt{\det M}}\left(M^{-1}\right)_{np}. \tag{2.17}$$

Propagator will just be element of inverse. Find with Fourier transforms.

$$\phi_n = \int_{-\pi}^{\pi}\frac{\mathrm{d}^4k}{(2\pi)^4}e^{ik\cdot n}\phi_k \tag{2.18}$$

$$S = \frac{1}{2}\sum_{n,p}\int\frac{\mathrm{d}^4k\mathrm{d}^4q}{(2\pi)^8}e^{i(k\cdot n+q\cdot p)}\phi_k\phi_q M_{np} \tag{2.19}$$

M is full of Kronecker deltas, so the sum collapses. We can combine exponentials except for the hopping terms, leaving

$$S = \frac{1}{2}\sum_n\int_{k,q}e^{i(k+q)\cdot n}\phi_k\phi_q\left[m^2+\sum_\mu[2-e^{iq_\mu}-e^{-iq_\mu}]\right] \tag{2.20}$$

Note that

$$2 - e^{iq_\mu} - e^{-iq_\mu} = 2(1 - \cos q_\mu) = 4\sin^2\frac{q_\mu}{2} \tag{2.21}$$

$$\hat{k}_\mu \equiv 2\sin\left(\frac{k_\mu}{2}\right). \tag{2.22}$$

Now we've got a diagonal Fourier form of the action and it's clear that

$$G(n,p) = \int_{-\pi}^{\pi} \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{e^{ik\cdot(n-p)}}{m^2 + \sum_\mu \hat{k}_\mu^2}, \tag{2.23}$$

which is cosmetically similar to the Feynman propagator in the ctm (albeit because we named things really suggestively). Note that our lattice momentum $\hat{k}_\mu$ does not look a lot like $k_\mu = k_\mu^{\text{phys}}a$. However, this is a nice example because the continuum limit is straightforward. We want to hold m^{phys} and k^{phys} fixed in our limit process. At small a,

$$\hat{k}_\mu \to 2\frac{k^{\text{phys}}a}{2} = k^{\text{phys}}a, \tag{2.24}$$

so we get

$$a^2 G(n,p) = \frac{1}{a^2}\int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{e^{ik^{\text{phys}}\cdot(x-y)}}{\left(m^{\text{phys}}\right)^2 + \sum_\mu \left(k_\mu^{\text{phys}}\right)^2} \tag{2.25}$$

which is exactly what my suggestive notation promised it would be (Brillouin zone grows to all momenta). In general, we are less lucky. In an interacting theory the mass term will not be a physical mass that we know to hold fixed and there is more work to do.

(3) Reflection Positivity/Getting Back

Alluded earlier to difficulty of getting a valid Minkowski theory out of Euclidean solutions. We saw just now that we may even have difficulty getting back to ctm Euclidean theory from lattice. Focus on the first part. How do we go from Euclidean correlators to a physical QFT?

Well, in practice, we usually don't do it. However, we have an interest in whether or not it's possible to validate our work. The answers we want come from the Osterwalder–Schrader Theorem. First, what does "physical" mean?

- **(a)** Hilbert space of states with positive-definite norm
- **(b)** Hermitian Hamiltonian with spectrum bounded below
- **(c)** Unitary operators implementing Poincaré invariance

According to O–S, the price of this is

- **(a)** S_E invariant under the 4-D Euclidean group: $SO(4)$ plus translations
- **(b)** Symmetric Euclidean correlation functions (for bosons)
- **(c)** Reflection positivity

These first two merit consideration (esp. since we break Euclidean symmetry going to lattice), but the third is the meat. What on earth is reflection positivity? Analogous to unitarity.

Suppose we have a full set of Euclidean correlation functions $G_n(x_1,\ldots,x_n)$ (called Schwinger functions in axiomatic field theory). Define the Euclidean time-reversal operator θ by

$$(\vec{x},x_4)\xrightarrow{\theta}(\vec{x},-x_4). \tag{3.1}$$

Further, consider a space of test functions $f_j(x_1,\ldots,x_j)$ whose defining properties are

- Support only when $(x_k)_4 \geqslant 0$ for all arguments
- Falls off when arguments large (possibly compact support req'd?).

We say that our Euclidean theory satisfies reflection positivity if

$$\sum_{j,k}\int \mathrm{d}x_1\cdots\mathrm{d}x_j\mathrm{d}y_1\cdots\mathrm{d}y_k f_j^*(x_1,\ldots,x_j)f_k(y_1,\ldots,y_k)G(\theta x_1,\ldots,\theta x_j,y_1,\ldots,y_k)\geqslant 0 \tag{3.2}$$

for all sets of f_j and f_k such that the integrals converge. This is scary, but it's often either easy to show or show a counterexample. Why is this a reasonable thing to demand? Consider a 2-point function that we know comes from a Minkowski theory with physical Hamiltonian $\hat{H}$. Then

$$G(\theta x,y)=\langle 0|\hat{\phi}(\vec{y},0)e^{-\hat{H}y_4}e^{\hat{H}(-x_4)}\hat{\phi}(\vec{x},0)|0\rangle\,, \tag{3.3}$$

so if we have reflection positivity, considering specifically test functions with support only at $x_4 = y_4 = 0$,

$$\langle 0|\int \mathrm{d}^3y f_1(\vec{y})\hat{\phi}(\vec{y},0)\int \mathrm{d}^3x f_1^*(\vec{x})\hat{\phi}(\vec{x},0)\,|0\rangle\geqslant 0, \tag{3.4}$$

and we can read the left half as the dual of the right half. The right half is a superposition of field operators acting on the vacuum, so a physical state. Then this statement is exactly a statement of positive norm.

(a) Lattice reflection positivity

Need to define RP on the lattice. We have two choices for the what the reflection operator θ means: site-reflection or link-reflection. Site-reflection treats $n=0$ as the center of reflection, taking $n_4\to -n_4$ for each site. Link-reflection treats first link as center, taking $n_4\to 1-n_4$. We must satisfy reflection positivity under *both* conditions to meet the hypotheses of the O–S theorem!

What is RP on the lattice?

Our correlators look like

$$G=\frac{1}{Z}\int_\phi e^{-S}\phi_{n_1}\phi_{n_2}\cdots\phi_{n_j} \tag{3.5}$$

$$F=\sum_k\sum_{\{n_i\}}f_k(n_1,\ldots,n_k)\phi_{n_1}\cdots\phi_{n_k} \tag{3.6}$$

Then reflection positivity looks like

$$\frac{1}{Z}\int_{\phi} e^{-S} F\Theta F \geqslant 0, \tag{3.7}$$

where $\Theta(f(x)\phi(x)) = f^{*}(x)\phi(\theta x)$.

Problem is, there are a lot of appealing lattice schemes that violate one or both of these types. Some approaches to fermions lose link RP, and using next-nearest-neighbor derivatives breaks both kinds! The latter case gives complex energies when we continue back to a Minkowski Hamiltonian.

Fact is, *most* modern lattice techniques exhibit this issue. Are we wasting our time? No. According to "the lore", which is borne out by numerical results, all energies which are complex have real part near the cutoff $1/a$, far from the domain of low-energy phenomena that we want to inspect.

(4) Wrap-Up

We've looked at development of lattice field theory through Euclidean path integrals for a real scalar field, building on previous week's discussion of PI in QM. We've seen several examples of steps that are easy to do and hard to undo, which will be a theme in future talks. Next week will begin working toward things we care about by introducing gauge fields on the lattice.