An introduction to Lattice Quantum Chromodynamics

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Abstract

1 Introduction

The aim of this paper is to give a hands-on introduction to the how one can go from a rudimentary understanding of quantum mechanics and quantum field theory, to simulating quantum chromodynamics on the lattice. In order to kick this is of, let us begin by discussing our end-goal, Quantum Quantum Chromodynamics(QCD).

QCD is the theory for interacting quarks and gluons. It has since its inception gotten a reputation notoriously difficult to work with, much because it is not linear due to its three- and four-vertex gluon self interactions. This makes solving it rather difficult, and in our search for understanding this theory we come to embrace lattice QCD.

The Lattice QCD machinery is at its core a application of the Metropolis algorithm on solving path integrals. LQCD may at first glance seem familiar to the much simpler Ising model, but in contrast to the Ising model there are many more tools which need to be mastered and understood. Questions such as how to create a discretized field theory, how to analyze sparse datasets or parallelize code requiring communication between nodes will all be addressed in due time. The first step will be to understand the path integral formalism. Since this is a quantum theory, we will refresh ourselves on some basic quantum mechanics.

If the reader feels so inclined, feel free to skip to chapter about the Path Integral Formalism.

2 Refreshing quantum mechanics

2.1 The postulates of quantum mechanics

Let us begin by recapitulating the postulates of quantum mechanics. Depending on what literature you are looking at, a different number of postulates will be listed [Shankar [1], Griffiths [2], Laurent Nottale [3]]. However, let us start by looking at those which count as the most fundamental ones, and expand upon them[1].

I *Complex state function.* The state of a quantum mechanical system can be described by a complex valued vector, $|\psi\rangle$ that lives in Hilbert space $\mathcal{H}$. Vectors in Hilbert space is often referred to as states.

II *The correspondence principle.* A physical observable has an Hermitian operator. For every dynamical variable in classical mechanics, there is a corresponding quantum mechanical one. Further, the principle states we reproduce the classical results in the limit of large quantum numbers. Further, on order to convert to from classical to quantum mechanics, we replace the Poisson brackets with the the commutator ones divided by $i\hbar$.

$$\{\cdot,\cdot\} \to \frac{1}{i\hbar}[\cdot,\cdot] \tag{1}$$

Further, any observable $\hat{\Omega}$ measured will result in a eigenvalue ω associated with the observable. These are related through the equation eigenvalue equation, $\hat{\Omega}|\psi\rangle = \omega|\psi\rangle$

III *Von Neumann's postulate(collapse of state).* If we measure a system $|\psi\rangle$ with an observable Λ and get the eigenvalue of ω_i, then the system will be in a state $|\psi_i\rangle$ after the measurement[2]. We say that the system has *collapsed* into state $|\psi_i\rangle$.

IV *The Schröedinger equation.* We require a state vector $|\psi(t)\rangle$ to abide by the Schröedinger equation,

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \tag{2}$$

[1] If one wants to, there are actually three subsets of postulates in QM[see laurent nottale], the fundamental ones, the secondary ones which can be derived from the fundamental ones, and the principles which are more consequences of the fundamental ones.

[2] A measurement is here an ideal experiment which we minimally disturb the system and it is in compliance with theory. In classical mechanics, an ideal measurement is a measurement in which the system remains unaffected.

where the Hamiltonian $\hat{H}$ is a linear Hermitian operator constructed accordingly to the correspondence principle.

V *Born's postulate.* The wave function squared $|\psi|^2$ is interpreted as a the probability of the system at a given configuration. For instance, the Probability of getting the eigenvalue ω_i in a state $|\psi\rangle$ is given by $|\langle\omega_i|\psi\rangle|^2$. This implies that the wave function must be normalized,

$$\langle\psi|\psi\rangle = 1 \tag{3}$$

From these postulates follow several other properties and consequences.

2.2 Formalism of Quantum mechanics

As alluded to in the postulates, the quantum mechanical world is on of vectors and Hilbert spaces. The rules of this game are built on top of properties that follows from the Hilbert space.

2.2.1 Superposition principle

Applying the superposition principle in quantum mechanics, we get from the linearity of the Hamiltonian $\hat{H}$ in the Schröedinger equation (2) that a quantum mechanical state is built up from a set of linear independent states. Given vectors $|u\rangle, |w\rangle \in \mathcal{H}$(which are our wave functions) and complex numbers α, β, we have that $\mathcal{H}$ is closed under addition and multiplication with scalars,

$$|w\rangle = \alpha|u\rangle + \beta|v\rangle \in \mathcal{H} \tag{4}$$

2.2.2 Adjoint operator

Further, we have that the inner product maps the vectors to complex numbers. From this we have the property of complex conjugate operators,

$$\langle u|v\rangle = \langle v|u\rangle^* \tag{5}$$

The inner product also adheres to the distributive property of complex numbers,

$$\langle w|\alpha u + \beta v\rangle = \alpha\langle w|u\rangle + \beta\langle w|v\rangle \tag{6}$$

2.2.3 Expansion in eigenfunctions

A state $|u\rangle$ can be expanded in a basis of eigenfunctions $|u_n\rangle \in \mathcal{H}$ as

$$u = \sum_n c_n |u_n\rangle \tag{7}$$

We demand orthogonality form this set, such that

$$\langle u_n | v_m \rangle = \delta_{nm} \tag{8}$$

2.2.4 Completeness relation

The unit operator 1 is given by

$$1 = \sum_n |u_n\rangle\langle u_n| \tag{9}$$

2.3 Operators

An operator will map a vector $|u\rangle$ in Hilbert space onto another vector in Hilbert space,

$$|u\rangle \in \mathcal{H} \rightarrow \hat{\Omega}|u\rangle \in \mathcal{H} \tag{10}$$

The adjoint operator is defined by

$$\langle u|\hat{\Omega}|v\rangle = \langle v|\hat{\Omega}^\dagger|u\rangle^* \tag{11}$$

An operator is *self-adjoint* or *Hermitian* if $\hat{\Omega}^\dagger = \hat{\Omega}$.

2.3.1 Eigenvectors and eigenvalues

The egeinvector(or eigenstate) of an operator $|u\rangle$ is given by

$$\hat{\Omega}|u\rangle = \lambda|u\rangle \tag{12}$$

with λ being a complex number and the eigenvalue.

2.3.2 Expectation values

Given some observable $\hat{\Omega}$ and a system described by a normalized wave function ψ, we have that the expectation value of that is given as the mean value from statistics.

$$\begin{aligned}\langle\Omega\rangle &= \sum_i P(\omega_i)\omega_i = \sum_i |\langle\omega_i|\psi\rangle|^2\omega_i \\ &= \sum_i \langle\psi|\omega_i\rangle\langle\omega_i|\psi\rangle\omega_i \\ &= \sum_i \langle\psi|\omega_i|\omega_i\rangle\langle\omega_i|\psi\rangle \\ &= \sum_i \langle\psi|\hat{\Omega}|\omega_i\rangle\langle\omega_i|\psi\rangle \\ &= \langle\psi|\hat{\Omega}\cdot I|\psi\rangle\end{aligned}$$

We used that $I = \sum_i |\omega_i\rangle\langle\omega_i|$ and that the $\omega_i|\omega_i\rangle = \hat{\Omega}|\omega_i\rangle$. This gives us the expression for the expectation value,

$$\langle\Omega\rangle = \langle\psi|\hat{\Omega}|\psi\rangle \tag{13}$$

2.4 Probability interpretation

The probability for finding a particle at a position x(assume we are in position space) is given by a function $|\psi(x)|^2$, probability per unit length. This is called the *probability density*. The *probability amplitude* is given by $\psi(x)$. The probability for finding the particle between two positions x_1 and x_2 is given by $\int_{x_1}^{x_2} |\psi(x)|^2 dx$. The probability of finding a particle at position x over a series of experiments is given by $\langle\psi|x|\psi\rangle = \int^{\mathrm{R}} \psi^*(x)x\psi(x)dx$.

3 The path integral formalism

The path integral formalism saw its complete form in 1948 with the help of Richard Feynman [4](but was however conceptualized somewhat earlier). The concept is both intuitive and elegant, and forms the basis of modern quantum field theory.

3.1 Path integral formalism in quantum mechanics

As the path integral formalism was first applied to quantum mechanics, it serves as a natural starting point. In quantum mechanics one usually starts by finding the eigenvalues and eigenstates of the Hamiltonian,

$$H = \frac{p^2}{2m} + V(x),$$

and then proceeds to find the propagator $U(t)$. The basic idea of a path integral is to go directly to expressing the propagator $U(x,t;x_0,t_0)$. This propagator describes the dynamics of a state x_0 evolving into another state x. Informally, we may think if this as:

1. Draw all paths connecting (x_0,t_0) and (x,t).
2. Find the phase or action(which serves as a weight analogous to statistical mechanics) $S[x(t)]$ for each path $x(t)$.
3. The propagator can now be expressed as a sum of all paths written in an informal way,

$$U(x,t;x_0,t_0) = \sum_{\text{all paths}} e^{iS[x(t)]},$$

with A as a normalization constant.

From this simple idea, we can start by setting $t = t_1 - t_0$ and writing the sum of all paths as a integral of all possible paths.

$$U(x,t;x_0,t_0) = \int \mathcal{D}x(t) e^{iS[x(t)]}$$

The question of *how* we will evaluate the integral comes from the classical idea that one satisfies the principle of least action (or the stationary condition [3]),

$$\frac{\delta}{\delta x(t)} \left(S\left[x(t)\right] \right) \Big|_{\text{cl}} = 0$$

with $S = \int dt L$ as the classical action. If we now assume that $S \gg \hbar$, we get our quantum mechanical path integral,

$$U(x_1,x_0,t) = \langle x_1 | \exp\left(-\frac{i}{\hbar} H t\right) |x_0\rangle = \int \mathcal{D}x(t) e^{iS[x(t)]/\hbar} \tag{14}$$

The idea of the path integral will be omnipresent in all of our calculations in Lattice QCD, and we will keep coming back to it in later chapters.

[3] See introduction in chapter 9 in [5]

3.2 Definition of the propagator

3.3 Euclidean path integrals

3.4 Correlation functions

3.5 Wick rotations

3.6 The Euclidean picture

3.7 Observables for the path integral

3.8 Switching between the Heisenberg and Schröedinger picture.

4 The Metropolis algorithm

5 Statistical analyses

What is autocorrelation? Autocorrelation versus correlation?

5.1 Bootstrapping

5.2 Jackknife method

5.3 Autocorrelation

5.4 Blocking

6 Quantum Field Theory and its fundamentals

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References

[1] Ramamurti Shankar. *Principles of quantum mechanics*. Springer US, 1994.

[2] David Griffiths. *Introduction of Quantum Mechanics*. Pearson Education Limited, 2013.

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[4] R. P. Feynman. Space-time approach to non-relativistic quantum mechanics. *Rev. Mod. Phys.*, 20:367–387, Apr 1948.

[5] D.V. Schroeder M.E. Peskin. *An Introduction to Quantum Field Theory*. Westview Press, 1995.