Monte Carlo Path Integration in QFT

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Canonical Quantisation

Canonical quantisation is a procedure that gets us from the classical Hamiltonian description of a system to a quantum mechanical one.

The Poisson bracket structure of classical mechanics morphs into the commutation relations between operators.

x_i – generalised coordinate

p_i – generalised momentum

$\{x_i, x_j\} = 0, \{p_i, p_j\} = 0$

$\{x_i, p_j\} = \delta_{ij}$

$H = H(\vec{q}, \vec{p}; t)$

$\dot{q}_i = \frac{\partial H}{\partial p_i}, \ \dot{p}_i = -\frac{\partial H}{\partial q_i}$

$\xrightarrow[\text{quantisation}]{\text{canonical}}$

$\hat{x}_i$ – position operator

$\hat{p}_i$ – momentum operator

$[\hat{x}_i, \hat{x}_j] = 0, [\hat{p}_i, \hat{p}_j] = 0$

$[\hat{x}_i, \hat{p}_j] = i\delta_{ij}$

$\hat{H}$ = hamiltonian operator

$i\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$

Quantum fields I

Quantisation of fields

In field theory we do the same, but starting from the classical field $\phi_i(\vec{x})$ and its momentum conjugate $\pi^i(\vec{x}) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i}$.

Hamiltonian operator

The quantum states obey the same Schrodinger equation $i\frac{d|\psi\rangle}{dt} = \hat{H}|\psi\rangle$ but with the hamiltonian $H = \int d^3x\, \mathcal{H}$, where the hamiltonian density $\mathcal{H}$ is obtained by a Legendre transform of the Lagrangian density $\mathcal{H} = \pi^i(x)\,\dot{\phi}_i(x) - \mathcal{L}(\phi, \partial_\mu \phi)$.

The quantum state $|\psi\rangle$

In QFT the notation $|\psi\rangle$ hides even more than in quantum mechanics, it depends of **every possible configuration of the field** ϕ.

Quantum fields II

Quantum Field

A quantum field is thus an operator valued function of space obeying the commutation relations:

$$\left[\hat{\phi}_i(\vec{x}), \hat{\phi}_j(\vec{y})\right] = \left[\hat{\pi}^i(\vec{x}), \hat{\pi}^j(\vec{y})\right] = 0$$
$$\left[\hat{\phi}_i(\vec{x}), \hat{\pi}^j(\vec{y})\right] = i\delta_i^j \delta^{(3)}(\vec{x} - \vec{y}).$$

Free fields I

Classical Klein-Gordon equation

The simplest classical relativistic free theory for a real scalar field $\phi(\vec{x}, t)$ is given by the Klein-Gordon equation $\partial_\mu \partial^\mu \phi + m^2 \phi = 0$. The most general solution is a linear superposition of independent simple harmonic oscillators at each point $\vec{p}$ in impulsion space $\phi(\vec{p}, t) = \mathcal{F}(\phi(\vec{x}, t))$.

Quantising the solution using a and $a^\dagger$ operators

When quantising the fields we will have an infinity of quantum harmonic oscillators at each point in momentum space. Recalling the solution to the harmonic oscillator in terms of destruction and creation operators we get:

$$\phi(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\omega_{\vec{p}}} \left[a_{\vec{p}} e^{i\vec{p}\cdot\vec{x}} + a^\dagger_{\vec{p}} e^{-i\vec{p}\cdot\vec{x}} \right]$$

$$\pi(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} (-i) \sqrt{\frac{\omega_{\vec{p}}}{2}} \left[a_{\vec{p}} e^{i\vec{p}\cdot\vec{x}} - a^\dagger_{\vec{p}} e^{-i\vec{p}\cdot\vec{x}} \right].$$

Free fields II

Free Field Quantum Hamiltonian

By substituting the ϕ and π field operators with their above expressions in the classical Klein-Gordon hamiltonian we obtain:

$$H = \int \frac{d^3p}{(2\pi)^3}\omega_{\vec{p}}\left[a^{\dagger}_{\vec{p}}a_{\vec{p}} + \frac{1}{2}(2\pi)^3\delta^3(0)\right].$$

The Vacuum

We define the vacuum $|0\rangle$ by saying it is annihilated by all $a_{\vec{p}}$:

$$a_{\vec{p}}|0\rangle = 0, \forall \vec{p}$$

Free fields III

Vacuum Energy

Applying H to the vacuum allows us to find its energy:

$$E_0 = \int d^3p \frac{1}{2}\omega_{\vec{p}}\delta^{(3)}(0) = \infty.$$

There are two divergences:

- infra-red divergence at large distances arising in $\delta^{(3)}(0)$. It can be remedied by putting the theory in a finite box.
- ultra-violet divergence at high frequencies arise due to the $|\vec{p}| \to \infty$ integral limits. This is because we assumed the theory is valid up to arbitrary energies, which is absurd. We can do a hight momentum cutoff. Alternatively, in this case, normal ordering leads to $E_0 = 0$.

Adding interactions I

Units

We are working with natural units $c = \hbar = 1$.
Since $[c] = LT^{-1} = [\hbar] = L^2MT^{-1} = 0$ all dimensionful quantities can be written in terms of a single mass/energy scale.
We denote $[X] = M^a lpha$ by $[X] \equiv \alpha$.

Lagrangian

Consider the general Lagrangian density with ϕ a scalar field in d dimensional space:

$$\mathcal{L} = \frac{1}{2}\partial_\mu\phi\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \sum_{n\geq 3}\frac{\lambda_n}{n!}\phi^n.$$

Given $[S] = [\hbar] = 0$ we have:
$[\mathcal{L}] = d, \quad [\partial_\mu] = 1, \quad [\phi] = 1, \quad [m] = 1, \quad [\lambda_n] = d - n.$

Adding interactions II

When are corrections small?

The dimensionless parameter is $\lambda_n E^{n-d}$ with E the relevant energy scale of the problem. As such, in our 4 dimensional space, corrections are small when $\lambda_n \ll E^{4-n}$:

- $n = 3$ terms are small at high energy $E \gg \lambda_3$ and big at low energy when $E \ll \lambda_3$
- $n = 4$ terms have dimensionless coupling constant $[\lambda_4] = 0$
- $n \geq 5$ terms are big at high energy $E \gg \lambda_3$ and small at low energy when $E \ll \lambda_3$

Most everyday physics happens at low energy (as far as particle physics is concerned) so that $n \geq 5$ terms are not important. Furthermore, parity symmetry ($x \to -x$) will also suppress $n = 3$ terms in the Lagrangian, when it is relevant.

Path Integral in Quantum Mechanics

Propagator

The path integral formulation places the propagator at the center of quantum mechanics and expresses it as a functional integral over paths:

$$\langle x_f | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | x_i \rangle = \left(\prod_{k=1}^{N-1} \int \mathrm{d}x_k \right) \prod_{j=1}^{N} \int \frac{\mathrm{d}p_j}{2\pi\hbar} e^{\frac{i}{\hbar}\Delta t \sum_{l=1}^{N} \left(p_l \frac{x_l - x_{l-1}}{\Delta t} - H(x_l, p_l) \right)}$$

$$= \int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}[x] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}\tau \; pv - H} = \int_{x(t_i)=x_i}^{x(t_f)=x_f} \mathcal{D}[x] e^{\frac{i}{\hbar}S[x]}$$

Wave Function

Using the propagator we can calculate wave functions:

$$\psi(x,t) = \langle x | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | \psi_i \rangle = \int \mathrm{d}x_i \, \langle x | \, e^{-\frac{i}{\hbar}\hat{H}t} \, | x_i \rangle \, \langle x_i | \psi_i \rangle$$

Free Propagator

Asking what is the probability to find a particle at point x (in 4D spacetime) after it has been prepared at point y leads us (as before) to the free (vacuum) propagator:

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

By imposing that the ϕ operators are *time ordered* we obtain the Feynman propagator which can be written as:

$$\Delta_F(x) = \int \frac{d^4p}{(2\pi)^4} \frac{ie^{-ip\cdot x}}{p^2 - m^2 + i\epsilon}.$$

Path Integral in QFT II

Field Sources

The language of boundary conditions used before (i.e. $x(t_i) = x_i$) is no longer appropriate in field theory where particles are created, interact and destroyed. As such what we are interested in most of the time is the *vacuum-to-vacuum transition amplitude in the presence of a source* (denoted Z). The source $J(x)$ is represented by modifying the Lagrangian:

$$\mathcal{L} \longrightarrow \mathcal{L} + J(x)\,\phi(x).$$

Generating Functional for Scalar Fields

By substituting $\mathcal{D}x \to \mathcal{D}\phi$ we can define the vacuum-to-vacuum transition amplitude within the path integral approach:

$$Z[J] = \int \mathcal{D}\phi \exp\left\{ i \int d^4 \left[\mathcal{L}(\phi) + J(x)\,\phi(x) + \frac{i}{2}\epsilon\phi^2 \right] \right\}.$$

Monte Carlo Path Integration I

A QFT on a lattice

In lattice field theory we discretise the number of field degrees of freedom to a finite lattice in d dimensions with N^d sites: $\phi(x) \to [\phi] = \{\phi_n\}$, with n taken to be the index of a lattice site.

Expectation Values

Using the generating functional we can write the time-ordered vacuum expectation value of a functional F as:

$$\langle F \rangle = \frac{\int \mathcal{D}\phi \; F[\phi] e^{iS[\phi]}}{\int \mathcal{D}\phi \; e^{iS[\phi]}} \approx Z^{-1} \int \prod_{j=1}^{N^d} d\phi_j e^{-S[\phi]} F[\phi]$$

where we used the Wick rotation to go to Euclidian path integrals in imaginary time.

Monte Carlo Path Integration II

Sample Average

Due to the immense number of integration variables the only numerical approach available is Monte Carlo simulation. The numerical task is to generate samples consisting of a large number of field lattice configurations $\{\phi_n\}$ that follow the distribution $e^{-S[\phi]}$. For a sample with γ configurations the average of F would then be:

$$\bar{A} = \frac{1}{\gamma} \sum_{n=1}^{\gamma} A[\phi_n].$$

Monte Carlo Path Integration III

Lattice Action

The expression we obtain for the action of a scalar d-dimensional field theory is:

$$S[\phi] = \int d^d x \left(\frac{1}{2} \partial_\mu \partial^\mu \phi + U(\phi) \right) \rightarrow \sum_{n=1}^{N^d} \left[\frac{1}{2} \sum_{\mu} (\phi_{n+\mu} - \phi_n)^2 + U(\phi) \right]$$

where μ signifies sum over sites neighboring site n. Note also that the expression on the right is adimensional and must be multiplied by a dimensional constant for physical interpretation.

Monte Carlo Path Integration IV

Metropolis Algorithm

Starting from some field configuration update each site as follows:

1. Generate some new value of the field ϕ_n at site n using a random number.
2. Calculate the lattice action difference ΔS
3. Keep or discard the change as follows:
   - if $\Delta S > 1$ keep it
   - if $\Delta S < 1$ keep it with probability ΔS.
4. Go to the next site

A ϕ^4 real scalar theory

Lagrangian

Consider a real scalar field theory with Lagrangian:

$$\mathcal{L} = \frac{1}{2}\partial_\mu \partial^\mu \phi + m^2 \phi + g\phi^4$$

on a 2D lattice.

Numerical Simulation

For the study of this particular theory I wrote a computer program in python that implemented the Metropolis algorithm previously discussed. In order to verify that the results make sense I compared the value of $\langle \phi^2 \rangle$ given by the simulation with a result obtained from perturbation theory by numerical integration.

$\langle\phi\rangle$ for a 40x40 lattice

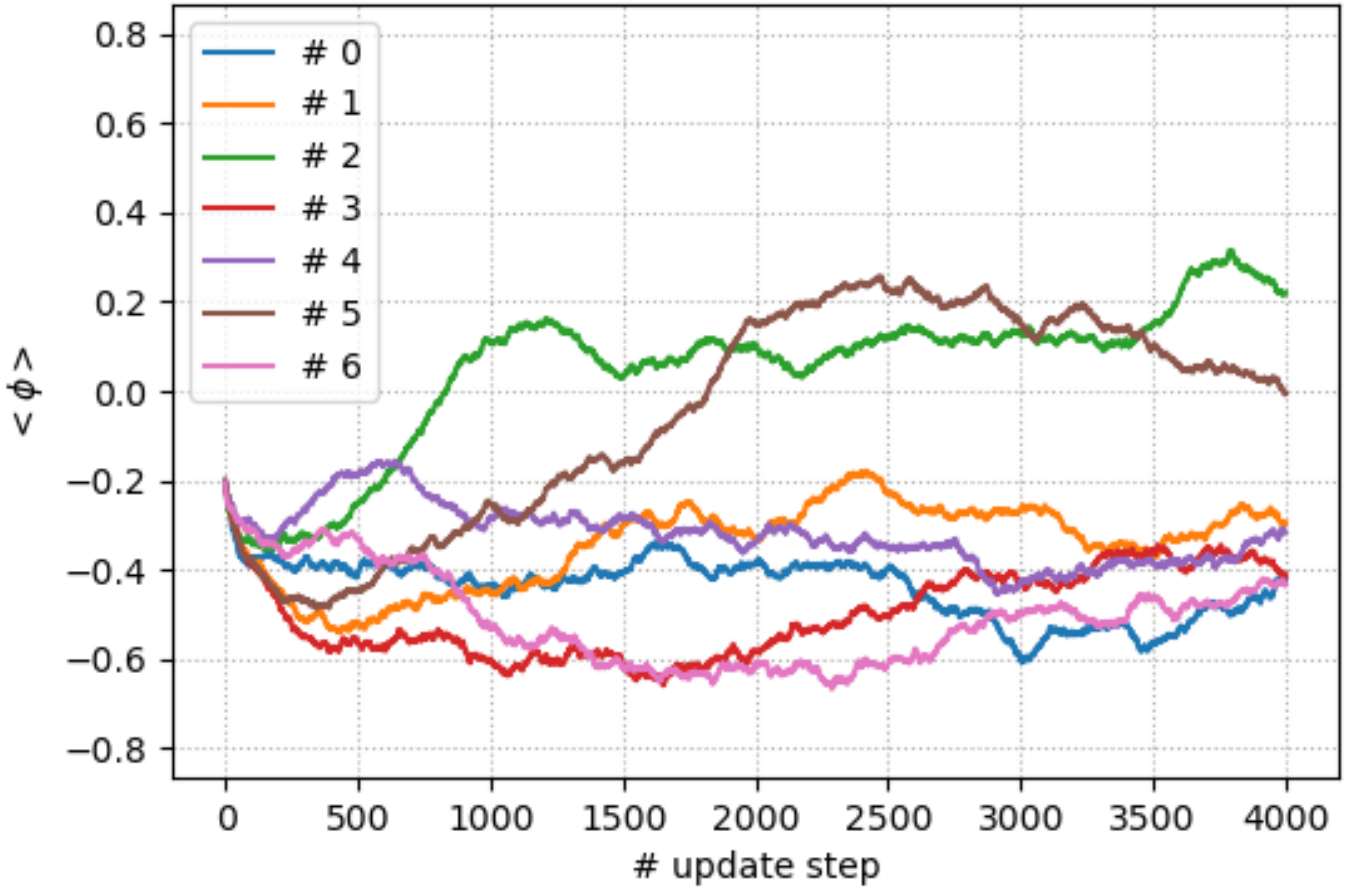

Figure: The average value of the field configuration as the simulation progresses. As expected the value hovers around 0. $m^2 = 2 \quad g = 1$

$\langle \phi^2 \rangle$ for a 40x40 lattice

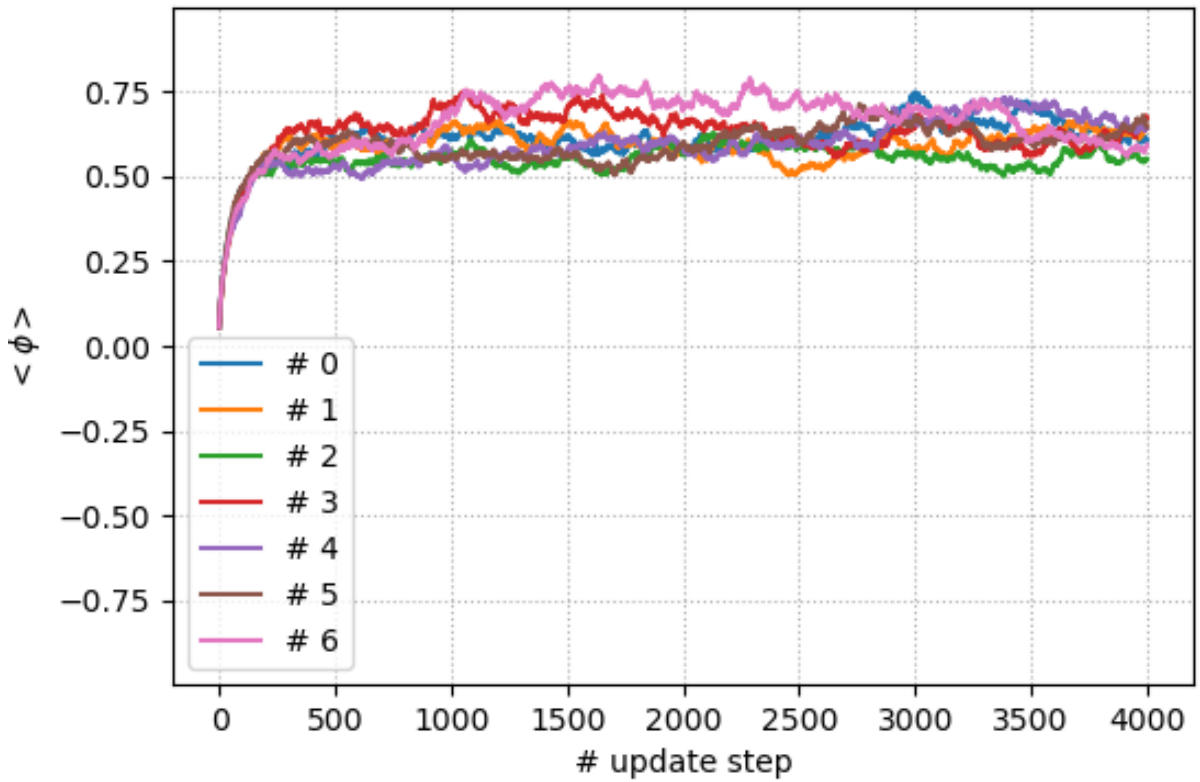

Figure: The average value of the field squared per configuration as the simulation progresses. The exact result is $\langle \phi^2 \rangle = 0.60$, it is to be compared with the theoretical calculated value of $\langle \phi^2 \rangle_{th} \approx 0.3$ The difference is a factor of 2.
$m^2 = 2 \quad g = 1$

Phase Structure I

Field Theory and Statistical Physics

The Wick Rotation establishes a link between the canonical ensemble statistical physics ($Z = \sum e^{\beta H}$) and field theory ($Z = \int \mathcal{D}\phi e^{iS}$). Because in the path integral formulation the operators disappear completely there is an equivalence between a **quantum field theory** in d spacial dimensions and a **classical statistical system** in $d+1$ spacial dimensions.

Connection to Landau Theory

Landau Theory is a generic recipe for the study of phase transitions:

1. Define an order parameter ψ
2. Assume a free energy functional $\tilde{F} = F_0(T) + F_L(T, \psi)$
3. Construct $F_L(\psi)$ as an analytic function of ψ obeying all symmetries of the system.

Phase Structure II

Link to Paramagnetism

The numerical calculations done via the path integral amount to calculating the exact functional integral from the Landau expansion of a paramagnetic system. Studying the relation between $\langle\phi\rangle$ and the Lagrangian parameters g and m^2 informs us about phase structure.

Phase Structure III

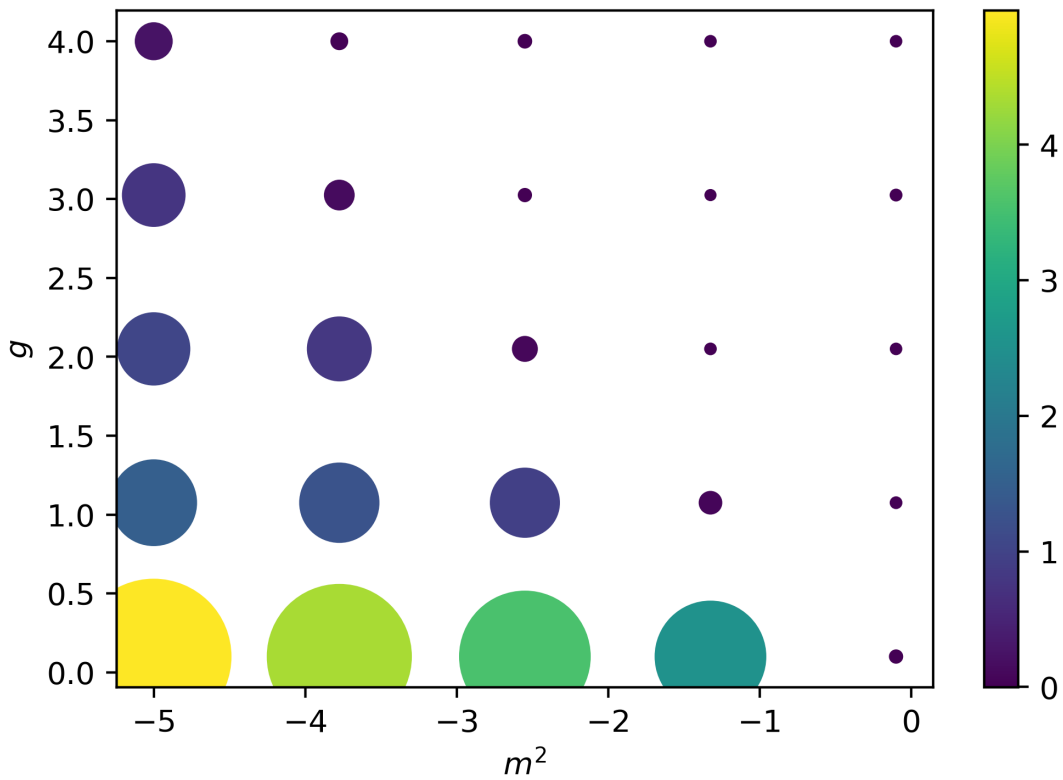

Figure: The horizontal and vertical axes represent m^2 and g parameters respectively. The size and color encode the value of $\langle\phi\rangle$. We can see a transition from a symmetric phase on the right to a broken phase on the left.

Conclusion

- The Monte Carlo path integration is a unique tool that allows us to explore quantum field theories in a non perturbative way.
- There is a profound link between Quantum Field Theory and Statistical Physics via the Path Integral.
- Time and computational constrains resulted in the exploration of only the simplest quantum field theory possible.

Questions