Abstract

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(Something about the fact that in the strong coupling case we cannot apply perturbation theory. It depends on what I will write in the general introduction)

2.1 Quantum field theory and statistical mechanics

We can build a non-perturbative tool for quantum field theory by exploiting the strong similarity between quantum field theory and statistical mechanics. This gives us the possibility of applying Monte Carlo simulations, an intrinsically non-perturbative method, to quantum field theory.

In the path-integral formulation of quantum field theory, the generating functional of correlation functions is defined as:

$$Z[J] = \int \mathcal{D}\phi \exp\left[i \int \mathrm{d}^4x \left(\mathcal{L}[\phi] + J(x)\phi(x)\right)\right] , \tag{2.1}$$

where ϕ generically represents the field content of the theory, $\mathcal{L}$ is the Lagrangian and $J(x)$ is an external source field. n-point functions are obtained by applying the functional derivative $\delta/\delta J(x)$ to $Z[J]$ as follows:

$$\begin{aligned} \langle 0|\, \mathrm{T}\phi(x_1)\ldots\phi(x_n)\,|0\rangle =& \frac{1}{Z[0]} \prod_{i=1}^{n} \left(-i\frac{\delta}{\delta J(x_i)}\right) Z[J]\bigg|_{J=0} = \\ =& \frac{1}{Z[0]} \int \mathcal{D}\phi\, \phi(x_1)\ldots\phi(x_n) \exp\left[i\int \mathrm{d}^4x\, \mathcal{L}[\phi]\right] , \end{aligned} \tag{2.2}$$

where $|0\rangle$ represents the vacuum state and T the time-ordered product. By performing a Wick rotation, we can make the generating functional 2.1 to be formally equal to the partition function of a statistical mechanical model.

As a concrete example, we consider a complex scalar field theory, with action:

$$S[\phi,\phi^*] = \int \mathrm{d}^4x\, \mathcal{L}[\phi,\phi^*] = \int \mathrm{d}^4x \big(\partial_\mu\phi^*\partial^\mu\phi - m^2|\phi|^2 - \lambda|\phi|^4\big) , \tag{2.3}$$

and generating functional:

$$Z[J,J^*] = \int \mathcal{D}\phi\mathcal{D}\phi^* \exp\left[iS[\phi,\phi^*] + i\int \mathrm{d}^4x\, J^*(x)\phi(x) + i\int \mathrm{d}^4x\, \phi^*(x)J(x)\right] . \tag{2.4}$$

After performing a Wick rotation ($x^0 = -ix^0_E$, $x^i = x^i_E$), the following changes occur:

$$\begin{aligned} i\mathrm{d}^4x &= \mathrm{d}^4x_E \\ \partial_\mu\phi^*\partial^\mu\phi &= -\delta_{\mu\nu}\partial^\mu_E\phi^*\partial^\nu_E\phi . \end{aligned} \tag{2.5}$$

We define the Euclidean action as:

$$S_E[\phi,\phi^*] = \int \mathrm{d}^4x_E \big(\delta_{\mu\nu}\partial^\mu_E\phi^*\partial^\nu_E\phi + m^2|\phi|^2 + \lambda|\phi|^4\big) , \tag{2.6}$$

and we find that the generating functional

$$Z[J,J^*] = \int \mathcal{D}\phi\mathcal{D}\phi^* \exp\left[-\left(S_E[\phi,\phi^*] - \int \mathrm{d}^4x_E J(x_E)\phi(x_E) - \int \mathrm{d}^4x_E J^*(x_E)\phi^*(x_E)\right)\right] \tag{2.7}$$

is now formally equal to the partition function of a statistical mechanical system.

2.2 Monte Carlo simulations

In statistical mechanics, the probability for a system in thermal equilibrium to be found in the microscopical configuration ϕ is given by:

$$P[\phi] = \frac{e^{-H[\phi]/k_B T}}{Z} , \tag{2.8}$$

$Z = \sum_\phi \exp[-H[\phi]/k_B T]$ being the partition function, $H[\phi]$ the total energy of the system in the configuration ϕ, k_B the Boltzmann constant and T the temperature. Monte Carlo simulations are a numerical method for generating configurations distributed according to the probability distribution $P[\phi]$.

In the previous section, we argued that a quantum field theory, defined by the action $S[\phi]$, is equivalent to a statistical mechanical model with partition function

$$Z = \int \mathcal{D}\phi\, e^{-S_E[\phi]} \tag{2.9}$$

(here for simplicity we consider the case of zero external source). We can apply the Monte Carlo method for generating configurations distributed according to:

$$P[\phi] = \frac{e^{-S_E[\phi]}}{Z} . \tag{2.10}$$

Once we have an ensemble of such configurations, n-point functions are calculated by averaging products of fields over the configurations:

$$\frac{1}{Z}\int \mathcal{D}\phi\, \phi(x_1)\dots\phi(x_n)e^{-S_E[\phi]} \longrightarrow \frac{1}{N}\sum_{i=1}^{N}\phi_i(x_1)\dots\phi_i(x_n)\ , \tag{2.11}$$

where $\phi_i(x_j)$ is the value of the field ϕ at the space-time point x_j, in the i-th configuration.

In order to construct a Monte Carlo simulation, we consider a stochastic process generating a sequence of configurations. We start from an initial configuration ϕ_0 at "Monte-Carlo time" (MC-time) $t = 0$, and move to a new configuration ϕ_1 with transition probability $W(\phi_0 \to \phi_1)$. The following normalisation condition holds for the transition probability W:

$$\sum_{\phi'} W(\phi \to \phi') = 1\ . \tag{2.12}$$

We repeat this procedure many times, thus generating a sequence of configurations. The probability $P[\phi; t]$ of being in the configuration ϕ at MC-time t fulfils the following condition:

$$P[\phi; t] = \sum_{\phi'} P[\phi'; t-1]W(\phi' \to \phi)\ . \tag{2.13}$$

We want the stochastic process to have the Boltzmann distribution $P_B[\phi] = \exp[-S_E[\phi]]/Z$ as an attractive fixed point. This means that, after some thermalisation time t_T, the probability distribution stops changing with MC-time, and it equals the Boltzmann distribution: $P[\phi; t > t_T] = P_B[\phi]$. If we are able to build such a stochastic process, then we can obtain an ensemble of Boltzmann-distributed configurations on which we can apply equation 2.11 for calculating n-point functions.

It follows from equation 2.13 that, if P_B is a fixed point of the stochastic process, then:

$$P_B[\phi] = \sum_{\phi'} P_B[\phi']W(\phi' \to \phi)\ . \tag{2.14}$$

We define the detailed-balance relation as:

$$P_B[\phi]W(\phi \to \phi') = P_B[\phi']W(\phi' \to \phi)\ ; \tag{2.15}$$

this relation implies the fixed-point condition 2.14 (this can be shown by summing equation 2.15 over ϕ', and using the normalisation condition 2.12), and it is easier to verify in a specific stochastic process. A process satisfying the detailed balance relation can be parametrised as follows:

$$W(\phi \to \phi') = F\left(\frac{P_B[\phi']}{P_B[\phi]}\right)\ , \tag{2.16}$$

where F is a generic function satisfying the functional equation

$$\frac{F(z)}{F(1/z)} = z\ . \tag{2.17}$$

There are many possible choices for the function F, each of whom defines a viable algorithm for a Monte Carlo simulation. One of the most widely used is $F(z) = \min[1, z]$, leading to the transition probability:

$$W(\phi \to \phi') = \min\left[1, \frac{P_B[\phi']}{P_B[\phi]}\right] = \min\left[1, e^{-(S_E[\phi'] - S_E[\phi])}\right] . \tag{2.18}$$

This particular implementation of the Monte Carlo method is known as Metropolis algorithm [1].

The stochastic process described above can be implemented numerically. To make this possible, we must define the theory on a lattice of finite volume, so that each field configuration is represented by a discrete and finite set of real numbers. Specifically, one configuration is completely defined by the value of each field at each point of the discretised space-time. In section 2.3 we will discuss the definition of a gauge theory on a space-time lattice.

To conclude, Monte Carlo simulations are a powerful non-perturbative method for studying quantum field theories. The price to be paid is the introduction of different sources of error that must be carefully treated: discretisation errors, finite-volume effects and statistical errors due to conducting the analysis on a finite set of configurations.

2.3 Lattice action

As previously pointed out, in order to apply the Monte Carlo method to a quantum field theory, we must first define the theory on a discretised space-time. In this section we discuss the lattice discretisation of a gauge theory coupled to fermions.

We define the discretised space-time as the set of points:

$$\Lambda = \{\, x_\mu = n_\mu a \mid n_\mu = 0, \ldots, L_\mu - 1,\ \mu = 0, \ldots, 3 \,\} , \tag{2.19}$$

where a is the lattice spacing and L_μ the number of lattice points in direction μ. We denote by $\hat{\mu}$ the unit vector in direction μ. As discussed in section 2.1, we are interested in defining the theory on a Euclidean space-time . However, for some purposes (such as measuring masses via the exponential falloff of correlators) it is useful to maintain the notion of time direction on the lattice. We consider $\mu = 0$ as time direction, i.e. the one that must be Wick-rotated in order to analytically continue the Euclidean theory to Minkowski space.

When we define a quantum field theory on a lattice with a finite number of points, the functional integral becomes the product of a finite number of ordinary integrals. For example, in the case of a real scalar field theory we have:

$$\int \mathcal{D}\phi \to \int_{-\infty}^{\infty} \prod_{x \in \Lambda} \mathrm{d}\phi_x , \tag{2.20}$$

where ϕ_x is the value of the field ϕ at the lattice point x.

2.3.1 Gauge action

We consider a theory with SU(N) gauge symmetry, whose continuum action is defined in equations (?)(?). In order to define a discretised version of this theory, we assign to each link on the lattice Λ an element of the gauge group:

$$U_\mu(x) = \exp\Big[iagA^b_\mu(x)T^b\Big] \in \mathrm{SU(N)} \,, \tag{2.21}$$

where T^b, $b \in [1, \ldots, \mathrm{N}^2 - 1]$, are the generators of the fundamental representation of SU(N) and g is the gauge coupling. The following relation holds for the link variables U_μ:

$$U_{-\mu}(x) = U_\mu(x - a\hat{\mu})^\dagger \,. \tag{2.22}$$

We define a gauge transformation by assigning to each lattice site an independent element of the gauge group, $\Omega(x) \in \mathrm{SU(N)}$, and transforming the link variables as follows:

$$U_\mu(x) \to U'_\mu(x) = \Omega(x)U_\mu(x)\Omega(x + a\hat{\mu})^\dagger \,. \tag{2.23}$$

The Wilson plaquette action [2] is the first proposed lattice discretisation of the Yang-Mills action. It is defined as:

$$S_W[U] = \frac{2\mathrm{N}}{g^2}\sum_{x\in\Lambda}\sum_{\mu<\nu}\Big[1 - \frac{1}{\mathrm{N}}\mathrm{Re}\,\mathrm{tr}[U_{\mu\nu}]\Big] \,, \tag{2.24}$$

where the plaquette $U_{\mu\nu}$ is the ordered product of the link variables around an elementary loop on the lattice:

$$U_{\mu\nu}(x) = U_\mu(x)U_\nu(x + a\hat{\mu})U_\mu(x + \hat{\nu})^\dagger U_\nu(x)^\dagger \,. \tag{2.25}$$

$S_W[U]$ is invariant under the gauge transformation 2.23, and, in the limit $a \to 0$, it reduces to the Euclidean Yang-Mills action. This can be shown by expanding the link variables 2.21 in powers of a, and by making use of the Baker-Campbell-Hausdorff formula for expanding the products of link variables:

$$e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\ldots} \tag{2.26}$$

where A and B are generic matrices, and we are omitting higher powers of the matrices in the right-hand side. Moreover, we can relate a finite difference on the lattice to a continuum derivative as follows:

$$A_\mu(x + a\hat{\nu}) - A_\mu(x) = a\,\partial_\nu A_\mu(x) + \mathcal{O}(a^2) \,. \tag{2.27}$$

We find:

$$S_W[U] = \frac{a^4}{2}\sum_{x\in\Lambda}\sum_{\mu,\nu}\mathrm{tr}\big[F_{\mu\nu}(x)^2\big] + \mathcal{O}(a^2) \underset{a\to0,V\to\infty}{\longrightarrow} \frac{1}{4}\int \mathrm{d}^4x\,(F^a_{\mu\nu})^2 = S^E_{YM}[A] \,, \tag{2.28}$$

where $V = \prod_{\mu=0}^{3} L_\mu$ is the total number of lattice points, μ and ν are Euclidean indices, and $F_{\mu\nu}$ is the field strength tensor, as defined in equation (?).

It must be noticed that, as we discretise the Yang-Mills action, the Poincaré symmetry of the continuum theory is reduced to the smaller group of symmetries of an hypercubic lattice. However, the discretised action that we defined has the remarkable property of being exactly gauge invariant even at finite lattice spacing.

2.3.2 Fermion action

The continuum Dirac action in Euclidean space is defined by:

$$S_D^E[\psi, \bar{\psi}, A] = \int \mathrm{d}^4x\, \bar{\psi}(\not{D} + m\mathbb{1})\psi = \int \mathrm{d}^4x\, \bar{\psi}\left[\gamma_\mu^E(\partial_\mu + igA_\mu) + m\mathbb{1}\right]\psi\,, \quad (2.29)$$

where $\mathbb{1}$ is the identity matrix in Dirac space, and γ_μ^E are the Euclidean gamma matrices, related to the Minkowskian ones by: $\gamma_0^E = \gamma_0$, $\gamma_j^E = -i\gamma^j$ $(j = 1, 2, 3)$. In the following we will omit the superscript E, and it will be understood that, whenever we are discussing a lattice model, gamma matrices assume their Euclidean form.

We start by discretising in the most naive way the free-fermion action. We define the forward and backward lattice derivatives as:

$$\begin{aligned} \nabla_\mu\psi(x) &= \frac{\psi(x + a\hat{\mu}) - \psi(x)}{a} \\ \nabla_\mu^*\psi(x) &= \frac{\psi(x) - \psi(x - a\hat{\mu})}{a}\,, \end{aligned} \quad (2.30)$$

and we use the symmetrised combination:

$$\frac{1}{2}(\nabla_\mu + \nabla_\mu^*)\psi(x) = \frac{\psi(x + a\hat{\mu}) - \psi(x - a\hat{\mu})}{2a} \quad (2.31)$$

in the definition of the lattice fermion action, which is:

$$S_F[\psi, \bar{\psi}] = a^4 \sum_{x\in\Lambda} \bar{\psi}(x)\left[\sum_{\mu=0}^{3} \gamma_\mu \left(\frac{\psi(x + a\hat{\mu}) - \psi(x - a\hat{\mu})}{2a}\right) + m\mathbb{1}\psi(x)\right]. \quad (2.32)$$

We rewrite equation 2.32 in the more compact form:

$$S_F[\psi, \bar{\psi}] = a^4 \sum_{x,y\in\Lambda} \bar{\psi}(x) D(x|y) \psi(y)\,, \quad (2.33)$$

where the Dirac operator $D(x|y)$ is defined as:

$$D(x|y) = \sum_{\mu=0}^{3} \gamma_\mu \frac{\delta_{y,x+a\hat{\mu}} - \delta_{y,x-a\hat{\mu}}}{2a} + m\mathbb{1}\delta_{x,y}\,. \quad (2.34)$$

This formulation of the lattice fermion action leads to the problem known as fermion doubling. In order to explicitly show what the problem is, we consider the Fourier transform of the Dirac operator:

$$\tilde{D}(p|q) = \frac{1}{V} \sum_{x,y\in\Lambda} e^{-ip\cdot x} D(x|y) e^{iq\cdot y} = \delta(p-q)\tilde{D}(q) \tag{2.35}$$

where

$$\tilde{D}(q) = \frac{i}{a} \sum_{\mu} \gamma_\mu \sin(q_\mu a) + m\mathbb{1} \,. \tag{2.36}$$

See appendix A.2 for the definition of Fourier transforms on the lattice.

By inverting the operator in equation 2.36 and transforming back to coordinate space, we obtain the fermion propagator:

$$\langle \psi(x)\bar{\psi}(y)\rangle = D^{-1}(x|y) = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\mathrm{d}^4 q}{(2\pi)^4} e^{iq\cdot(x-y)} \frac{m\mathbb{1} - i/a\sum_\mu \gamma_\mu \sin(q_\mu a)}{m^2 + \sum_\mu \sin^2(q_\mu a)/a^2} \,. \tag{2.37}$$

Here for simplicity we consider the infinite-volume limit, where lattice momenta have a continuum spectrum. In the limit $a \to 0$, the dominant contributions to the integral 2.37 arise from momentum ranges where

$$\frac{1}{a}\sin(q_\mu a) \sim 0 \,. \tag{2.38}$$

This happens around $q = (0,0,0,0), (\pi/a,0,0,0), \ldots, (\pi/a,\pi/a,\pi/a,\pi/a)$. Of all these contributions, only the one arising from the integration around $q = (0,0,0,0)$ corresponds to the continuum propagator

$$\langle \psi(x)\bar{\psi}(y)\rangle_{\text{cont}} = \int_{-\infty}^{\infty} \frac{\mathrm{d}^4 q}{(2\pi)^4} e^{iq\cdot(x-y)} \frac{m\mathbb{1} - i/a\sum_\mu \gamma_\mu q_\mu}{m^2+q^2} \,, \tag{2.39}$$

while the other fifteen contributions have no continuum analogue, and are not defined in the continuum limit. These are lattice artefacts known as doublers.

One of the possible solutions to the doubling problem is to add an extra term to the Dirac operator, known as Wilson term [3]. The Wilson-Dirac operator in momentum space is defined by:

$$\tilde{D}(q) = \frac{i}{a}\sum_\mu \gamma_\mu \sin(q_\mu a) + m\mathbb{1} + \mathbb{1}\frac{1}{a}\sum_\mu \big(1-\cos(q_\mu a)\big) \,, \tag{2.40}$$

leading to the fermion propagator:

$$\langle \psi(x)\bar{\psi}(y)\rangle = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{\mathrm{d}^4 q}{(2\pi)^4} e^{iq\cdot(x-y)} \frac{\big[m + a^{-1}\sum_\mu\big(1-\cos(q_\mu a)\big)\big]\mathbb{1} - ia^{-1}\sum_\mu \sin(q_\mu a)}{\big[m + a^{-1}\sum_\mu\big(1-\cos(q_\mu a)\big)\big]^2 + a^{-2}\sum_\mu \sin^2(q_\mu a)} \,. \tag{2.41}$$

We define $q^{(\pi)}$ as a momentum vector with n_π components equal to π/a and the other $4-n_\pi$ components equal to zero. In the vicinity of $q^{(\pi)}$, the denominator in equation 2.41 is given by:

$$\left[m+\frac{1}{a}\sum_\mu\big(1-\cos(q_\mu a)\big)\right]^2+\frac{1}{a^2}\sum_\mu \sin^2(q_\mu a)\underset{q\sim q^{(\pi)}}{\sim}\left[m+\frac{2n_\pi}{a}\right]^2+\frac{1}{a^2}\sum_\mu \sin^2(q_\mu a)\,. \tag{2.42}$$

This expression is finite in the $a \to 0$ limit only if $n_\pi = 0$, otherwise it diverges. Thus the contributions from the doublers are eliminated. The price to be paid is that the Wilson fermion action is not chirally symmetric in the limit $m \to 0$.

The Wilson term $\tilde{D}_W(q) = \mathbb{1}a^{-1}\sum_\mu\big(1-\cos(q_\mu a)\big)$ has the following form in coordinate space:

$$D_W(x|y) = -\mathbb{1}a\sum_\mu \frac{\delta_{y,x+a\hat{\mu}}-2\delta_{x,y}+\delta_{y,x-a\hat{\mu}}}{2a^2}\underset{a\to 0}{\to} -\mathbb{1}\frac{a}{2}\partial_\mu\partial_\mu\,. \tag{2.43}$$

Equation 2.43 shows that D_W is a discretisation of the Laplace operator $\partial_\mu\partial_\mu$, multiplied by a factor a, which makes it clear that the Wilson term goes to zero in the limit of vanishing lattice spacing.

We now introduce the gauge interaction by inserting link variables in the products of neighbouring fermion fields:

$$\begin{aligned}&\bar{\psi}(x)\psi(x+a\hat{\mu}) \to \bar{\psi}(x)U_\mu(x)\psi(x+a\hat{\mu})\\ &\bar{\psi}(x)\psi(x-a\hat{\mu}) \to \bar{\psi}(x)U_{-\mu}(x)\psi(x-a\hat{\mu}) = \bar{\psi}(x)U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})\,.\end{aligned} \tag{2.44}$$

Now the fermion fields carry a colour index along with the Dirac index, and they transform as:

$$\begin{aligned}\psi(x) &\to \Omega(x)\psi(x)\\ \bar{\psi}(x) &\to \bar{\psi}(x)\Omega^\dagger(x)\end{aligned} \tag{2.45}$$

under the gauge transformation 2.23, which shows that the products defined in equation 2.44 are gauge invariant.

To conclude, the interacting Wilson-Dirac operator is given by:

$$D(x|y) = \left(m+\frac{4}{a}\right)\mathbb{1}\times\mathbb{1}_C\delta_{x,y}-\frac{1}{2a}\left[\sum_\mu(\mathbb{1}-\gamma_\mu)U_\mu(x)\delta_{y,x+a\hat{\mu}}+\sum_\mu(\mathbb{1}+\gamma_\mu)U_\mu^\dagger(x-a\hat{\mu})\delta_{y,x-a\hat{\mu}}\right]. \tag{2.46}$$

where $\mathbb{1}_C$ represents the identity matrix in colour space.

We have thus defined Wilson's formulation of a lattice gauge theory coupled to fermions. The action is given by:

$$S[U,\psi^{(i)},\bar{\psi}^{(i)}] = \frac{2\mathrm{N}}{g^2}\sum_{x\in\Lambda}\sum_{\mu<\nu}\big[1-\frac{1}{\mathrm{N}}\mathrm{Re}\,\mathrm{tr}[U_{\mu\nu}]\big]+\sum_{i=1}^{N_f}a^4\sum_{x,y\in\Lambda}\bar{\psi}^{(i)}(x)D^{(i)}(x|y)\psi^{(i)}(y)\,, \tag{2.47}$$

where $U_{\mu\nu}$ is the plaquette, defined in equation 2.25, $D(x|y)$ is the Wilson-Dirac operator defined in equation 2.46, and N_f is the number of fermion flavours. The partition function of this model is:

$$Z = \int \prod_{x\in\Lambda} \left[\prod_{\mu} \mathrm{d}U_\mu(x) \right] \left[\prod_i \mathrm{d}\psi^{(i)}(x) \mathrm{d}\bar{\psi}^{(i)}(x) \right] e^{-S[U,\psi^{(i)},\bar{\psi}^{(i)}]} \,, \tag{2.48}$$

where $\mathrm{d}U_\mu(x)$ is the Haar measure for the integration over the gauge group.

The action 2.47 is not a unique choice. There exist other formulations, which for example have smaller discretisation errors, or implement a lattice version of chiral symmetry in the fermion action. For the study described in this thesis, Wilson's formulation 2.47 is used.

2.3.3 Pseudofermions

Fermion fields are represented in the path integral formalism by anticommuting Grassmann variables. Unfortunately, it is not possible to define Grassmann variables on a computer. This problem can be solved by using following trick: the Gaussian integral over the fermion fields is explicitly calculated:

$$\int \prod_{x\in\Lambda} \mathrm{d}\psi(x) \mathrm{d}\bar{\psi}(x) \exp\left[- \sum_{x,y\in\Lambda} \bar{\psi}(x) D(x|y) \psi(y) \right] = \det[-D] \,, \tag{2.49}$$

and then the fermionic determinant $\det[-D]$ is rewritten as an integral over new bosonic variables, known as pseudofermions.

But first of all it must be shown that the fermions' contribution to the partition function is real and nonnegative. The minus sign inside the determinant is actually irrelevant, since it simply provides an overall factor $(-1)^N$ in front of the path integral, where N is the dimension of the matrix D. If $\det[D]$ is a nonnegative real number in each gauge configuration, then it can be seen as a part of the Boltzmann weight in the partition function

$$Z = \int \prod_{x\in\Lambda} \left[\prod_{\mu} \mathrm{d}U_\mu(x) \right] \det[D] e^{-S_W[U]} \,, \tag{2.50}$$

otherwise it cannot be interpreted as probability density.

The Wilson-Dirac operator is γ_5-hermitian: $\gamma_5 D = D^\dagger \gamma_5$. We can use this property for defining an hermitian operator:

$$Q = \gamma_5 D \,, \tag{2.51}$$

whose determinant is a real number. Since $\det[\gamma_5] = 1$, the determinants of D and Q are equal, implying that the determinant of the Wilson-Dirac operator is real. But this does not guarantee that $\det[D]$ is nonnegative.

A possible strategy for ensuring the positivity of the integrand in the partition function is to have couples of mass-degenerate fermion fields in the theory. Two mass-degenerate fermions are coupled to identical Dirac operators, and contribute to the partition function with a factor $\det[D]^2 \geq 0$.

We can now define the lattice fermion action in terms of pseudofermion fields.We consider a theory with two mass-degenerate fermions, and we rewrite the fermionic contribution as an integral over bosonic degrees of freedom, ϕ and $\phi^\dagger$:

$$\det[D]^2 = \det[Q]^2 = \det\big[Q^2\big] = \pi^{-N} \int \prod_{x\in\Lambda} \mathrm{d}\phi(x)\mathrm{d}\phi^\dagger(x) \exp\Big[-\sum_{x,y\in\Lambda} \phi^\dagger(x)Q^{-2}(x|y)\phi(y)\Big]. \tag{2.52}$$

The factor π^{-N} can be neglected, since it is an overall factor in the path integral. The lattice action can now be expressed as a function of bosonic variables:

$$S[U,\phi,\phi^\dagger] = \frac{2\mathrm{N}}{g^2}\sum_{x\in\Lambda}\sum_{\mu<\nu}\big[1-\frac{1}{\mathrm{N}}\mathrm{Re}\,\mathrm{tr}[U_{\mu\nu}]\big]+a^4\sum_{x,y\in\Lambda}\phi^\dagger(x)Q^{-2}(x|y)\phi(y)\,, \tag{2.53}$$

and is suitable for the implementation of a Monte Carlo simulation.

2.4 Hybrid Monte Carlo

The lattice action 2.53 is highly nonlocal, due to the inverse Q operator in the pseudofermion term. It may be inefficient in this case to use algorithms based on local updates of the configurations. By local update we mean that just one or a few link variables are changed when generating a new configuration.

For example, we imagine to update the gauge field by changing the value of one link variable, and then to accept or reject the new configuration according to Metropolis transition probability 2.18. Even though only one link variable has been changed, the variation of the action appearing in equation 2.18 depends on all the link variables in the lattice. With this method, subsequent configurations are highly correlated to each other, and at the same time each Metropolis step is computationally expensive.

In this case it is a better solution to change all the link variables at once. The Hybrid Monte Carlo (HMC) algorithm is based on the idea of updating the configurations via a molecular dynamics evolution, in such a way that all the link variables are changed, but at the same time the change in the action is very small, so that the new configuration is very likely to be accepted in a Metropolis step. In this section we describe the general idea behind the HMC method by using a scalar field theory as a concrete example. In section 3.3.2 we will give the details for the application of the method to a gauge theory coupled to fermions and scalars.

We consider a scalar field theory, with action $S[\phi]$, and we write the expectation value of an observable O as:

$$\langle O\rangle = \frac{\int\prod_x \mathrm{d}\phi(x)\,O[\phi]\exp[-S[\phi]]}{\int\prod_x \mathrm{d}\phi(x)\ \exp[-S[\phi]]} = \frac{\int\prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x)\,O[\phi]\exp\Big[-\frac{1}{2}\sum_y\pi(y)^2 - S[\phi]\Big]}{\int\prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x)\ \exp\Big[-\frac{1}{2}\sum_y\pi(y)^2 - S[\phi]\Big]}, \tag{2.54}$$

where in the last step we multiplied both numerator and denominator by the factor $\int \prod_x \mathrm{d}\pi(x) \exp\left[-\frac{1}{2}\sum_y \pi(y)^2\right]$. We interpret $H[\pi,\phi] = \frac{1}{2}\sum_x \pi(x)^2 + S[\phi]$ as an Hamiltonian, whose Hamilton's equations are given by:

$$
\begin{aligned}
\dot{\pi}(x) &= -\frac{\partial H}{\partial \phi(x)} = -\frac{\partial S}{\partial \phi(x)} \\
\dot{\phi}(x) &= \frac{\partial H}{\partial \pi(x)} = \pi(x) \, ,
\end{aligned}
\tag{2.55}
$$

where the dot denotes the derivative with respect to molecular-dynamics time. If we were able to exactly solve these equations, we would have a trajectory in configuration space characterised by a constant value of the Hamiltonian.

The HMC method is based on solving numerically Hamilton's equations 2.55, thus generating a molecular dynamics trajectory. The system is let evolve for a finite number of steps of the numerical integrator and the final configuration is accepted or rejected in a Metropolis step, with acceptance probability

$$
W_M(\pi, \phi \to \pi'\phi') = \min\left[1, \frac{e^{-H[\pi',\phi']}}{e^{-H[\pi,\phi]}}\right] . \tag{2.56}
$$

In appendix A.3 we show that, when the numerical integrator meets certain requirements, the algorithm described above respects the detailed balance relation 2.15.

To conclude, the HMC algorithm is very useful for simulating gauge theories coupled to dynamical fermions. It reduces the correlation between subsequent configurations in the Monte Carlo evolution, and at the same time the acceptance can be kept high by tuning the parameters of the numerical integrator.

2.5 Mass measurements on the lattice

Among the many interesting observables that can be measured on the lattice, there is the energy spectrum of the theory. The energy levels can be measured from the study of correlation functions.

We define the correlation function in Euclidean time of two generic operators A and B as:

$$
C_{AB}(t) = \langle A(t)B(0)\rangle = \frac{1}{Z}\,\mathrm{tr}\left[e^{-(T-t)\hat{H}} A(0) e^{-t\hat{H}} B(0)\right] , \tag{2.57}
$$

where the partition function Z is expressed in the operator formalism as:

$$
Z = \mathrm{tr}\left[e^{-T\hat{H}}\right] . \tag{2.58}
$$

$T \equiv L_0$ is the number of lattice points in the time direction, and $t \equiv x^0$ is the Euclidean time coordinate. $\hat{H}$ is the Hamiltonian operator generating time translations, and the trace is intended over the Hilbert space of physical states.

We choose a basis of eigenstates of $\hat{H}$, $\hat{H}\,|n\rangle = E_n\,|n\rangle$, and we rewrite equations 2.57 and 2.58 as:

$$C_{AB}(t) = \frac{1}{Z}\sum_n \langle n|\, e^{-(T-t)\hat{H}} A(0) e^{-t\hat{H}} B(0)\,|n\rangle \ , \tag{2.59}$$

$$Z = \sum_n \langle n|\, e^{-T\hat{H}}\,|n\rangle \ . \tag{2.60}$$

By inserting a completeness relation, $\sum_m |m\rangle\langle m| = \mathbb{1}$, we obtain:

$$\begin{aligned} C_{AB}(t) &= \frac{1}{Z}\sum_{n,m} \langle n|\, e^{-(T-t)\hat{H}} A(0)\,|m\rangle \langle m|\, e^{-t\hat{H}} B(0)\,|n\rangle = \\ &= \frac{\sum_{n,m} e^{-TE_n} e^{-t(E_m-E_n)} \langle n|\, A(0)\,|m\rangle \langle m|\, B(0)\,|n\rangle}{\sum_n e^{-TE_n}} \ . \end{aligned} \tag{2.61}$$

In the limit of large lattice time extent, $T \to \infty$, only the vacuum state contributes to the sum over n:

$$C_{AB}(t) \underset{T\to\infty}{\sim} \sum_m e^{-t(E_m-E_0)} \langle 0|\, A(0)\,|m\rangle \langle m|\, B(0)\,|0\rangle \ . \tag{2.62}$$

In the limit of large time separations, $t \to \infty$, only the lightest state with nonzero overlap with $B(0)\,|0\rangle$ and $A^\dagger(0)\,|0\rangle$ contributes to the sum over m:

$$C_{AB}(t) \underset{\substack{T\to\infty \\ t\to\infty}}{\sim} e^{-t(E_{m_0}-E_0)} \langle 0|\, A(0)\,|m_0\rangle \langle m_0|\, B(0)\,|0\rangle \ . \tag{2.63}$$

In this setup, the energy of the state $|m_0\rangle$ can be measured by studying the exponential decay of the correlator $C_{AB}(t)$ for large Euclidean time separations. The energy is measured with respect to the energy of the vacuum state E_0. The goal is then to find operators A and B with a good overlap with the states whose energy we want to to measure. In the following we describe the operators used for the mass measurements done in this thesis.

2.5.1 Meson masses

In order to measure meson masses, we need operators that generate states with the quantum numbers of the desired mesons. We consider a theory with two fermion flavours, and, in analogy with the first quark family of the Standard Model, we denote the fermion fields by u (up) and d (down). These two fermions belong to an isospin doublet, with $I = 1/2$, and $I_3 = +1/2$ (u), $I_3 = -1/2$ (d).

In this thesis we will measure the mass of the isospin-triplet pseudoscalar mesons (analogue to pions in QCD) and the isospin-triplet vector mesons (analogue to ρ mesons in QCD). For the pseudoscalar isospin triplet, the following operators are used:

- $(I = 1, I_3 = +1)$: $O_{\pi^+}(x) = \bar{d}(x)\gamma_5 u(x)$
- $(I = 1, I_3 = 0)$: $O_{\pi^0}(x) = \frac{1}{\sqrt{2}}\big(\bar{u}(x)\gamma_5 u(x) - \bar{d}(x)\gamma_5 d(x)\big)$

- $(I = 1, I_3 = -1)$: $O_{\pi^-}(x) = \bar{u}(x)\gamma_5 d(x)$.

These operators have spin zero and negative parity, O_{π^0} is an eigenstate of the charge conjugation operator, with eigenvalue $+1$, while O_{π^+} and O_{π^-} are mapped into each other by charge conjugation. When the fermion masses are degenerate and there are no electroweak interactions, the three states $\pi^{\pm,0}$ have the same mass, therefore it is sufficient to study only one of these operators.

In order to measure the mass of the pseudoscalar meson state, the correlator $C_{\pi^-}(t) = \sum_{\mathbf{x}} \langle O_{\pi^-}(\mathbf{x}, t) O^\dagger_{\pi^-}(\mathbf{0}, 0)\rangle$ is used in this thesis. The sum over the spacial coordinates $\mathbf{x}$ is introduced for projecting to states with zero spacial momentum. In fact, going back to equation 2.63, it can be seen that if there exists a one-particle state with the chosen quantum numbers, then the energy of the lowest-energy state with zero spacial momentum is simply given by the mass of the particle.

The operators chosen for studying the isospin-triplet vector mesons are very similar to $O_{\pi^\pm}$ and O_{π^0}, with the only difference that γ_5 is replaced with γ_i, $i = 1, 2, 3$. These operators generate states with spin one and negative parity. Again, in the absence of electroweak effects and if u and d have the same mass, the three states in the isospin triplet have equal masses.

2.5.2 PCAC mass

In this thesis we will also measure the fermion mass via the Partially Conserved Axial Current (PCAC) relation. The PCAC relation, or axial Ward identity, is a consequence of the transformation properties of the fermion action under chiral rotations in flavour space. In order to derive it, we consider the partition function 2.48, and a field redefinition:

$$\begin{aligned} \psi^{(i)} &\to \psi^{(i)} + \delta\psi^{(i)} \\ \bar{\psi}^{(i)} &\to \bar{\psi}^{(i)} + \delta\bar{\psi}^{(i)} \; . \end{aligned} \tag{2.64}$$

The partition function doesn't change under this transformation, and, if the integration measure is also symmetric, it follows that:

$$\langle \delta S \rangle = 0 \; , \tag{2.65}$$

where δS is the infinitesimal shift in the action.

We now consider the continuum fermion action for a two-flavour theory:

$$S_{\mathrm{cont}}[\psi, \bar{\psi}] = \int \mathrm{d}^4 x \, \bar{\psi}(x)(\gamma_\mu D_\mu + M\mathbb{1})\psi(x) \; , \tag{2.66}$$

where $\psi = (u \; d)^T$, M is the two-by-two diagonal mass matrix and $\mathbb{1}$ the identity in Dirac space. As in the previous section, we denote the two fermion fields by u and d. We consider the following infinitesimal transformation in flavour space:

$$\begin{aligned} \psi(x) &\to \psi(x) + i\epsilon(x)\gamma_5\sigma^a\psi(x) \\ \bar{\psi}(x) &\to \bar{\psi}(x) + i\epsilon(x)\bar{\psi}(x)\gamma_5\sigma^a \; , \end{aligned} \tag{2.67}$$

where σ^a are the Pauli matrices, with $a = 1, 2, 3$, and $\epsilon(x)$ is a generic smooth function, which is nonzero only inside a bounded region. For this specific transformation, equation 2.65 reads:

$$\langle \partial_\mu \big(\bar{\psi}(x) \gamma_\mu \gamma_5 \sigma^a \psi(x) \big) \rangle = \langle \bar{\psi}(x) \big\{ M, \sigma^a \big\} \gamma_5 \psi(x) \rangle \ . \tag{2.68}$$

If the two fermions have equal masses, $m_u = m_d = m$, equation 2.68 becomes:

$$\langle \partial_\mu A^a_\mu(x) \rangle = 2m \langle P^a(x) \rangle \ , \tag{2.69}$$

where we have defined the axial vector current as $A^a_\mu = 1/2 \, \bar{\psi} \gamma_\mu \gamma_5 \sigma^a \psi$, and the pseudoscalar interpolator as $P^a = 1/2 \, \bar{\psi} \gamma_5 \sigma^a \psi$. P^a is related to the $O_{\pi^{\pm,0}}$ operators of the previous section by:

$$\begin{aligned} P^1 - iP^2 &= \bar{d} \gamma_5 u = O_{\pi^+} \\ P^1 + iP^2 &= \bar{u} \gamma_5 d = O_{\pi^-} \\ P^0 &= \frac{1}{2} \big(\bar{u} \gamma_5 u - \bar{d} \gamma_5 d \big) = \frac{1}{\sqrt{2}} O_{\pi^0} \ . \end{aligned} \tag{2.70}$$

Equation 2.69 is known as PCAC relation, and it implies that, when $m = 0$, the axial vector current is conserved, due to the symmetry of the action under chiral flavour rotations. On the lattice however, the Wilson fermion action is not chirally symmetric even when the fermion mass is zero, and the analogue of the PCAC relation involves additional terms.

The PCAC relation can be used to measure the fermion mass on the lattice by studying the long-distance behaviour of the following ratio of correlators:

$$\frac{1}{2} \frac{\sum_{\mathbf{x}} \langle \partial_t A^-_0(\mathbf{x}, t)^\dagger O_{\pi^-}(0) \rangle}{\sum_{\mathbf{x}} \langle O_{\pi^-}(\mathbf{x}, t)^\dagger O_{\pi^-}(0) \rangle} \underset{t \to \infty}{\sim} m_{PCAC} \ , \tag{2.71}$$

where $A^-_\mu = A^1_\mu + iA^2_\mu$, and, due to the zero-momentum projection, only the time derivative survives. m_{PCAC} is identified with the unrenormalised fermion mass. Due to the fact that the lattice fermion action is not chirally symmetric, m_{PCAC} is not equal to the bare mass used as parameter in the fermion action, and in general is not zero when the bare mass is zero. The chiral limit of the lattice theory is identified by finding the values of the bare lattice parameters such that $m_{PCAC} = 0$.

2.6 The continuum limit

Lattice calculations make it possible to study non-perturbatively the discretised version of a quantum field theory. Information on the continuum theory can be obtained by performing the continuum limit.

We have previously observed that, in the limit $a \to 0$, the lattice action 2.47 reduces to the continuum Euclidean action of a gauge theory coupled to fermions. However, this is not enough to ensure that meaningful continuum results can be extracted from the lattice theory. In order to illustrate this, we consider the mass of some physical state, measured on the lattice from the exponential decay of a correlator, as described in section 2.5. The lattice calculation results in a dimensionless quantity $\hat{M}$, which is the inverse of a correlation length, and is related to the physical value of the mass M by: $M = \hat{M}/a$. If we want M to be finite in the continuum limit, we need $\hat{M}$ to go to zero as a goes to zero. This means that the bare parameters of the lattice theory must be tuned to a critical point, where correlation lengths diverge.

When we say that $M = \hat{M}/a$ is the physical value of the mass, we are implicitly assuming that we can express the lattice spacing a in physical units, say in fm. This information is not contained in the lattice theory itself, and it must be deduced by using some external input. For example, if we are studying lattice QCD, we can pick any observable, such as the mass of a bound state, and set its experimental value to be equal to the value measured on the lattice. From this equality we can extract the value of the lattice spacing measured in physical units.

Once we have a measure for the lattice spacing, the goal is to extrapolate continuum physics out of the lattice results by moving to smaller and smaller values of the lattice spacing. As pointed out earlier, in order to have finite values for the observables in the continuum limit, we have to change the bare lattice couplings as functions of a, in such a way that when a goes to zero we move towards a critical point where correlation lengths diverge. In particular, in a pure gauge theory the gauge coupling g must change as a function of a in such a way that:

$$O(a, g(a)) \underset{a\to 0}{\longrightarrow} O_{ph} \,, \tag{2.72}$$

where O is a generic observable and O_{ph} is its physical value. The functional form of $g(a)$ may depend on the specific observable if a is not small enough. However, when we get close to the continuum limit, there must be a unique function $g(a)$ that ensures the finiteness of any observable. We can obtain information on $g(a)$ by using the renormalisation group equation:

$$\left[a\frac{\partial}{\partial a} - \beta(g)\frac{\partial}{\partial g}\right] O(a, g(a)) = 0 \,, \tag{2.73}$$

where $\beta(a) = -a\, \partial g/\partial a$. We obtain this equation by assuming to be close enough to the continuum limit, so that equation 2.72 can be rewritten as an equality, and by deriving with respect to a the right- and left-hand-side. The beta function $\beta(g)$ can be computed perturbatively by expanding $O(a, g)$ in powers of g, and by inserting the expansion in equation 2.73. The result up to $\mathcal{O}(g^3)$ is the same for any observable O, and it is given by:

$$\beta(g) = -\frac{11N}{3}\frac{g^3}{(4\pi)^2} + \mathcal{O}(g^5) \,, \tag{2.74}$$

where we assumed the gauge group to be SU(N). With the help of equation 2.74, we can solve the differential equation $\beta(a) = -a\, \partial g/\partial a$ and express a as a function of g:

$$a = \frac{1}{\Lambda_L} e^{-\frac{(4\pi)^2}{2\beta_0 g^2}} \,, \tag{2.75}$$

where $\beta_0 = 11N/3$, and Λ_L is a constant with the dimension of an energy. Equation 2.75 shows that the lattice spacing goes to zero when g goes to zero, and therefore we have to move in parameter space towards $g = 0$ in order to take the continuum limit.

When studying a lattice gauge theory coupled to fermions, there is one extra parameter to consider: the fermion mass m. We consider here the case of Wilson fermions, whose action is defined in section 2.3.2, and we define the bare fermion mass measured in lattice units as $\hat{m} = ma$. The typical procedure for ensuring that in the continuum limit we describe the desired theory (for example QCD), is to repeat the lattice measurements for different values of g, and for each value of g to tune $\hat{m}$ in such a way that some dimensionless ratio of observables assumes its physical value. This way a line of constant physics in the space of bare lattice parameters is defined. The physical value of the lattice spacing is determined by equalling one observable to its experimental value, and then all the other observables can be expressed in physical units, representing the real independent lattice measurements. The continuum value of these observables is extrapolated by moving towards $g = 0$ along the line of constant physics.

One more important point to consider when taking the continuum limit is the lattice volume. As the lattice spacing becomes smaller, the number of lattice points must be increased, so that the physical volume doesn't shrink. Typically the extrapolation to $a = 0$ is performed by keeping the physical lattice volume fixed, which implies increasing the number of lattice points as $g \to 0$.

Chapter 3

Lattice study of a gauge-fermion-scalar theory

The Standard Model electroweak theory is very successful in describing experimental results. However, some theoretical concerns suggest that a more consistent theory should be found. Specifically, the search for an alternative mechanism for the generation of masses is an active research field. Composite Higgs models belong to this branch of Beyond the Standard Model (BSM) research.

In this chapter we discuss the lattice study of an SU(2) gauge theory coupled to fermions and scalars. This theory is intended as a minimal scenario for composite Higgs models, in which the problem of the generation of fermion masses is addressed via the fundamental partial compositeness mechanism [4].

The chapter is organised as follows. We start by exposing some of the reasons why the Standard Model Higgs mechanism turns out to be theoretically unappealing. Then we introduce composite Higgs models, and we explain what makes the generation of fermion masses a bit problematic in this setup. We then describe the mechanism of fundamental partial compositeness. After setting these theoretical motivations, we move to the description of the specific theory under analysis, starting with some continuum aspects and then moving to the lattice setup. Finally, we present the results obtained on the spectrum and phase space of the lattice theory.

3.1 Composite Higgs models and fundamental partial compositeness

3.1.1 The naturalness and triviality problems

The Standard Model Higgs boson is an elementary scalar field. There exist some theoretical problems related to elementary scalars, known as naturalness and triviality problem.

The naturalness problem is due to the fact that the Higgs mass is extremely sensitive to corrections arising from new physics, which may appear at a very high energy scale. We know the Standard Model to be an effective field theory, valid up to some ultraviolet cutoff Λ_{SM}, whose UV-completion is yet unknown. Λ_{SM} will be at most equal to the Planck scale $M_{PL} = 10^{19}$ GeV, where a complete quantum theory of gravity should appear. When we consider the Standard Model (SM) as an effective theory, we do not restrict ourselves to the renormalisable operators of the SM Lagrangian, but we consider an effective Lagrangian containing all possible operators built with the SM elementary fields, which respect the symmetries of the SM:

$$\mathcal{L}_{eff} = \sum_{d=1}^{\infty} \frac{c_{(d)}}{\Lambda_{SM}^{d-4}} O^{(d)} \;, \tag{3.1}$$

where d is the energy dimension of the operator $O^{(d)}$. For dimensional reasons, the coefficients of $d > 4$ operators are suppressed by a factor $\Lambda_{SM}^{-|d-4|}$, while the coefficients of $d < 4$ operators are enhanced by a factor $\Lambda_{SM}^{|d-4|}$. If we knew the UV-completion of the SM, i.e. a theory valid up to arbitrarily high energy scales, of which the SM is a low-energy effective description, then we could in principle compute the coefficients $c_{(d)}$ as functions of the parameters of the UV-complete theory. The quadratic term in the Higgs potential is the only $d < 4$ operator present in $\mathcal{L}_{eff}$, specifically it is a $d = 2$ operator. The tree-level Higgs mass is proportional to the coefficient of this operator. The fact that the Higgs is "light", together with the fact that new physics may come at a very high energy scale, contributes to creating a theoretically problematic scenario. If new physics appeared at a scale which is significantly larger than the TeV, then reconstructing the experimental value of 125 GeV for the Higgs mass would require the coefficient $c_{(2)}$ to be extremely small. As a consequence, the UV-completion accounting for the new physics would be constrained by the fact that $c_{(2)}$ must assume the required very small value. This scenario, in which the low-energy parameters of the theory constrain to a very high degree the UV-completion, defined at a much higher scale, is considered to be unnatural.

Elementary scalars may also be affected by the triviality problem [5]. This problem is related to the running of the scalar quartic self-coupling. In a pure scalar field theory, defined by the Lagrangian

$$\mathcal{L}[\phi] = \frac{1}{2}\partial_\mu\phi\,\partial^\mu\phi - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{4!}\phi^4 \;, \tag{3.2}$$

the renormalised quartic coupling at the momentum scale p, at lowest order in perturbation theory, is given by:

$$\bar{\lambda}(p) = \frac{\lambda_R}{1 - \frac{3}{16\pi^2}\lambda_R \log\frac{p}{\mu}} \;, \tag{3.3}$$

where λ_R is the renormalised coupling at the scale $p = \mu$. If $\lambda_R \neq 0$, there exists a finite momentum scale at which the renormalised coupling diverges, thus making the theory inconsistent. It seems that the only consistent theory is the noninteracting one, characterised by $\lambda_R = 0$. Should this be the case also for the SM Higgs field, the Higgs mechanism would be invalidated, since it is strongly based on the existence of the scalar self-interactions. This argument however does not directly apply to the SM Higgs scalar, since gauge and Yukawa interactions must be also taken into account in order to compute the running of λ. The quartic coupling of the SM

Higgs actually becomes negative at high energies, thus leading to problems related to the stability of the SM vacuum [6]. A scalar field theory is trivial whenever an ultraviolet fixed point for the quartic coupling is absent. In this case, the theory is ill-defined at high energies, unless the renormalised coupling is set to zero, thus eliminating scalar self-interactions. This supports the interpretation of the SM as an effective field theory, defined up to an ultraviolet cutoff, and discourages the introduction of elementary scalars in a UV-complete theory.

3.1.2 Composite Higgs models

Composite Higgs models constitute an alternative to the Higgs mechanism for the generation of masses, in which no elementary scalars are included. The first inspiration for composite Higgs models came from the fact that the Higgs vacuum expectation value is not the only source of electroweak symmetry breaking in the Standard Model. In fact, QCD pions contribute to the mass of the W and Z gauge bosons. This is due to the fact that electroweak symmetry is embedded in the chiral $\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$ symmetry of QCD, which is spontaneously broken by the strong dynamics.

It is shown in [7] that, in a theory with the SM gauge symmetry $\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y\times\mathrm{SU}(3)_C$, containing one family of massless quarks and no Higgs doublet, the electroweak gauge bosons become massive. Specifically, the $W^\pm$ bosons acquire a mass $M_W = (g/2)f_\pi \simeq 30\,\mathrm{MeV}$, where g is the $\mathrm{SU}(2)_L$ gauge coupling, and f_π the pion decay constant. Moreover, the photon is massless and the ratio of the W and Z masses is the same as in the SM. In order to obtain these results, the gauge couplings are assumed to run in the same way as in the SM. In particular, the $\mathrm{SU}(3)_C$ gauge coupling becomes ~ 1 at 1 GeV, and the electroweak sector is treated as a small perturbation. The tree-level value of $g/2$ can be deduced from the relation between the Fermi constant G_F and the W boson mass:

$$\frac{G_F}{\sqrt{2}} = \left(\frac{g}{2\sqrt{2}}\right)^2 \frac{1}{M_W^2}\,, \tag{3.4}$$

while the pion decay constant is given by $f_\pi = 93\,\mathrm{MeV}$ [8].

The W boson mass thus generated is clearly too small with respect to the experimental value of 80 GeV, and indeed in the SM the almost unique source of electroweak symmetry breaking is the Higgs vacuum expectation value. However, one may imagine a "scaled-up" version of QCD, where the pion decay constant is big enough to provide a realistic mass for W and Z bosons. This is the idea behind Technicolor (TC) models [9, 7]. In these models, all the SM particles are included except for the Higgs doublet, and on top of that a new strongly interacting sector is added. The new sector contains fermionic matter, which we will refer to as TC-fermions, and a new non-Abelian gauge interaction. The TC sector in isolation is symmetric under a global flavour symmetry, which is assumed to be spontaneously broken by the formation of the TC-fermion condensate. The flavour symmetry is required to have an $\mathrm{SU}(2)\times\mathrm{U}(1)$ subgroup, so as to allow the embedding of electroweak interactions. Specifically, the $\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y$ generators are identified with some of the broken generators of the TC flavour symmetry. As a consequence, the W and Z bosons acquire a mass proportional to the TC-pion decay constant. In these models the Higgs boson is identified with the lightest scalar resonance of the TC-sector. In general it is not automatic to obtain both a Higgs mass and W and Z masses in good agreement with experimental values. In particular, unless some care is taken, the Higgs boson will end up being heavier than the measured 125 GeV. Walking Technicolor models [10, 11, 12] address this kind of issue.

Another composite Higgs scenario is the one of composite Goldstone Higgs models [13, 14]. In these models a new strongly interacting sector analogous to the TC one is introduced (we will continue to call it TC sector), but the embedding of electroweak symmetry is substantially different. In fact, the $\mathrm{SU}(2)_L\times\mathrm{U}(1)_Y$ generators are identified with some of the unbroken generators of the TC flavour symmetry, so that W and Z bosons remain massless. The Higgs is identified with one of the Goldstone bosons of the broken flavour symmetry. Unless some explicit breaking of this symmetry is introduced, the Goldstone-Higgs is a massless particle. In order to generate the correct Higgs mass and to give masses to W and Z, some new interactions are introduced, which explicitly break the TC flavour symmetry. The explicit form of possible symmetry-breaking interactions will be discussed in the next section, in the case of a specific model. In the setup of composite Goldstone Higgs models, the Higgs boson is naturally light and a large separation occurs between the electroweak scale and the scale at which the TC gauge coupling becomes strong. Therefore the masses of non-Goldstone TC-hadrons are expected to be large with respect to the electroweak scale, and possibly beyond the range explored so far in accelerator experiments.

To conclude, we remark that in composite Higgs models electroweak symmetry is broken as a consequence of the dynamics of the theory. In this respect, these models are more theoretically satisfactory than the SM, where electroweak symmetry breaking is simply modelled and no dynamical reason is given for its occurrence. In the next section we analyse in some more detail the SU(2) gauge theory with two fermions in the fundamental representation, which can serve as setup for both Technicolor and composite Goldstone Higgs scenarios [15].

3.1.3 SU(2) + 2 fermions as minimal composite Higgs model

In this section, following the lines of [15], we discuss a specific model: the SU(2) gauge theory with two fermions in the fundamental representation. This is a good candidate for being the TC sector in both a Technicolor and a composite Goldstone Higgs scenario.

The Lagrangian of this model is given by:

$$\mathcal{L} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + \bar{u}(i\not{D} - m)u + \bar{d}(i\not{D} - m)d\,, \tag{3.5}$$

where u and d are the two TC-fermion fields with equal mass m, $F^a_{\mu\nu}$ is the non-Abelian field strength tensor and D_μ is the covariant derivative. In the case $m = 0$, this Lagrangian has a larger flavour symmetry than the $\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$ generally expected for an SU(N) gauge theory with two fundamental fermions. This is due to the fact that the fundamental representation of SU(2) is pseudo-real, i.e. there is a relation between a matrix of SU(2) and its complex conjugate:

$$U = (-i\sigma^2)U^*(i\sigma^2)\,, \quad U \in \mathrm{SU}(2)\,, \tag{3.6}$$

where σ^2 is the second Pauli matrix. Due to this property, we can define an enlarged flavour multiplet of left-handed fields transforming under the fundamental representation of SU(2):

$$Q = \begin{pmatrix} u_L \\ d_L \\ \tilde{u}_L \\ \tilde{d}_L \end{pmatrix}\,, \tag{3.7}$$

where the left- and right-handed spinors are defined by:

$$u_L = \frac{\mathbb{1}-\gamma_5}{2}u\,, \quad u_R = \frac{\mathbb{1}+\gamma_5}{2}u\,, \quad d_L = \frac{\mathbb{1}-\gamma_5}{2}d\,, \quad d_R = \frac{\mathbb{1}+\gamma_5}{2}d\,, \tag{3.8}$$

and we have defined some new left-handed fields $\tilde{u}_L$ and $\tilde{d}_L$ as:

$$\tilde{u}_L = -i\sigma^2 C\bar{u}_R^T\,, \quad \tilde{d}_L = -i\sigma^2 C\bar{d}_R^T\,. \tag{3.9}$$

In equation 3.9, the matrix $-i\sigma^2$ acts on the colour indices of the spinors, while C is the charge conjugation operator, acting on Dirac indices (see appendix A.1.2). As a consequence of equation 3.6, $\tilde{u}_L$ and $\tilde{d}_L$ transform under the fundamental representation of the TC group SU(2):

$$\begin{gathered} u_R \to u'_R = Uu_R, \quad U \in \mathrm{SU}(2) \\ \Downarrow \\ \tilde{u}'_L = -i\sigma^2 C\bar{u}'^T_R = -i\sigma^2 U^* C\bar{u}_R^T = U\tilde{u}_L\,. \end{gathered}$$

The Lagrangian 3.5 can be rewritten in terms of Q as follows:

$$\mathcal{L} = -\frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu} + i\bar{Q}\not{D}Q + \frac{m}{2}Q^T(-i\sigma^2)CEQ + \frac{m}{2}(Q^T(-i\sigma^2)CEQ)^\dagger\,, \tag{3.10}$$

where

$$E = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\,. \tag{3.11}$$

If $m = 0$, this Lagrangian is symmetric under global SU(4) transformations of the multiplet Q, while if $m \neq 0$ the symmetry is reduced to the subgroup Sp(4), defined as being the group of transformations such that the following condition is verified:

$$ET_n + T_n^T E = 0\,, \tag{3.12}$$

where T_n are the fifteen generators of the fundamental representation of SU(4).

After defining the TC sector in isolation, we embed electroweak symmetry by assigning the following transformation properties:

- $Q_L = (u_L, d_L)^T$ is an $\mathrm{SU}(2)_L$ doublet with zero hypercharge
- $\tilde{u}_L$ and $\tilde{d}_L$ are two $\mathrm{SU}(2)_L$ singlets with hypercharges -1/2 and +1/2 respectively.

With these assignments, we can identify the electroweak generators among the generators of flavour symmetry. First of all, we list the generators of SU(4), and, for future purposes, we split them into two groups, denoted by S^i, $i = 1, \ldots, 10$, and X^j, $j = 1, \ldots, 5$:

$$\begin{aligned} S^{1,2,3} &= \frac{1}{2}\begin{pmatrix} \sigma^i & 0 \\ 0 & 0 \end{pmatrix} , \quad S^{4,5,6} = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & -\sigma^{iT} \end{pmatrix} , \\ S^{7,8,9} &= \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & i\sigma^i \\ -i\sigma^i & 0 \end{pmatrix} , \quad S^{10} = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \end{aligned} \tag{3.13}$$

$$\begin{aligned} X^1 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & \sigma^3 \\ \sigma^3 & 0 \end{pmatrix} , \quad X^2 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} , \quad X^3 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix} , \\ X^4 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix} , \quad X^5 = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} , \end{aligned} \tag{3.14}$$

where, as usual, σ^i, $i = 1, 2, 3$, are the Pauli matrices. Due to the transformation properties of Q_L, $\tilde{u}_L$ and $\tilde{d}_L$ under the electroweak gauge group, $S^{1,2,3}$ are identified with the generators of $\mathrm{SU}(2)_L$, while S^6 is the generator of $\mathrm{U}(1)_Y$.

We now assume that the TC sector in isolation, in the SU(4)-symmetric case $m = 0$, undergoes spontaneous flavour symmetry breaking due to the formation of the TC-fermion condensate:

$$\langle Q^T(-i\sigma^2)C\Sigma_0 Q + (Q^T(-i\sigma^2)C\Sigma_0 Q)^\dagger \rangle \neq 0 \, . \tag{3.15}$$

The SU(4) flavour symmetry is broken down to the subgroup spanned by the unbroken generators, which fulfil the following condition:

$$\Sigma_0 T_n + T_n^T \Sigma_0 = 0 \, . \tag{3.16}$$

Σ_0 is a yet unspecified matrix in flavour space, whose alignment with respect to the electroweak generators will be determined by minimising the effective potential of the theory in interaction with the electroweak group, taking into account also possible symmetry-breaking perturbations.

We rewrite Σ_0 as the superposition:

$$\Sigma_0 = \cos\theta \, \Sigma_B + \sin\theta \, \Sigma_H \, , \tag{3.17}$$

where

$$\Sigma_B = \begin{pmatrix} i\sigma^2 & 0 \\ 0 & -i\sigma^2 \end{pmatrix} , \quad \Sigma_H = E = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix} . \tag{3.18}$$

If $\Sigma_0 = \Sigma_B$, the unbroken generators are the S^i's defined in equation 3.13, while the broken generators are the X^j's of equation 3.14. In particular, electroweak symmetry is preserved. If $\Sigma_0 = \Sigma_H$, the unbroken generators are:

$$S^1 + S^4\,, \quad S^2 + S^5\,, \quad S^3 + S^6\,, \quad S^{7,9,10}\,, \quad X^{1,2,3,5}\,, \tag{3.19}$$

and the broken ones:

$$S^1 - S^4\,, \quad S^2 - S^5\,, \quad S^3 - S^6\,, \quad S^8\,, \quad X^4\,. \tag{3.20}$$

In this case electroweak symmetry is broken. Moreover, we will see in the following that, for $\theta = \pi/2$, the mass of the $W^\pm$ bosons is directly determined by the Goldstone-boson decay constant and the $\mathrm{SU}(2)_L$ coupling constant, as in Technicolor models. It follows that a model with $\theta = \pi/2$ is a good candidate for Technicolor, while a model with $\theta \sim 0$ could work as composite Goldstone Higgs scenario.

For a generic alignment θ, the broken generators are given by the following combinations:

$$\begin{gathered} Y^1 = c_\theta X^1 - s_\theta \frac{S^1 - S^4}{\sqrt{2}}\,, \quad Y^2 = c_\theta X^2 + s_\theta \frac{S^2 - S^5}{\sqrt{2}}\,, \quad Y^3 = c_\theta X^3 + s_\theta \frac{S^3 - S^6}{\sqrt{2}}\,, \\ Y^4 = X^4\,, \quad Y^5 = c_\theta X^5 - s_\theta S^8\,, \end{gathered} \tag{3.21}$$

where $c_\theta = \cos\theta$ and $s_\theta = \sin\theta$. In order to study the phenomenology of the low-energy excitations of this model, the effective Lagrangian approach can be used. We define the Goldstone matrix as:

$$\Sigma = e^{i \frac{\phi^a}{f} Y^a} \Sigma_0\,, \tag{3.22}$$

where $\phi^a(x)$, $a = 1, \ldots, 5$, are the Goldstone boson fields and f the Goldstone boson decay constant. The kinetic term of the effective Lagrangian, where the electroweak interactions are introduced via the covariant derivative D_μ, is given by:

$$f^2 \,\mathrm{tr}\left[(D_\mu \Sigma)^\dagger D^\mu \Sigma\right]\,, \tag{3.23}$$

where

$$D_\mu \Sigma = \partial_\mu \Sigma - i(G_\mu^T \Sigma + \Sigma G_\mu)\,, \tag{3.24}$$

$$G_\mu = g W_\mu^i S^i + g' B_\mu S^6\,, \quad i = 1, 2, 3\,. \tag{3.25}$$

In the previous equation, g is the $\mathrm{SU}(2)_L$ coupling, g' the $\mathrm{U}(1)_Y$ coupling and W_μ^i, B_μ their respective gauge boson fields.

In [15], computations are carried on in the unitary gauge, i.e. by fixing to zero the Goldstone boson fields which provide the longitudinal degrees of freedom of W and Z. In our case this means: $\phi^{1,2,3} = 0$. The remaining Goldstone bosons are renamed as: $\phi^4 \equiv h$, $\phi^5 \equiv \eta$. The Goldstone matrix in the unitary gauge reads:

$$\Sigma = e^{\frac{i}{f}(h Y^4 + \eta Y^5)} \Sigma_0\,. \tag{3.26}$$

By inserting 3.26 in 3.23, and expanding in powers of η/f, h/f, one finds the masses and couplings of the fields $W^{\pm}$, Z, h and η. W^i and B are expressed in terms of $W^{\pm}$, A and Z as in equations (*must be added in the introduction*). The resulting gauge boson masses are:

$$m_W^2 = 2g^2 f^2 s_\theta^2 \,, \tag{3.27}$$

$$m_Z^2 = 2(g^2 + g'^2) f^2 s_\theta^2 = \frac{m_W^2}{\cos^2\theta_W} \,, \tag{3.28}$$

where θ_W is the Weinberg angle. The Goldstone bosons h and η are massless (at tree level), and their couplings to the electroweak gauge bosons are given by:

$$g_{hWW} = \sqrt{2} g^2 f s_\theta c_\theta = g m_W c_\theta = g_{hWW}^{SM} c_\theta \,, \tag{3.29}$$

$$g_{hZZ} = \sqrt{2}(g^2 + g'^2) f s_\theta c_\theta = \sqrt{g^2 + g'^2} m_Z c_\theta = g_{hZZ}^{SM} c_\theta \,, \tag{3.30}$$

$$g_{hhWW} = \frac{1}{4} g^2 c_{2\theta} = g_{hhWW}^{SM} c_{2\theta} \,, \tag{3.31}$$

$$g_{hhZZ} = \frac{g_{hhWW}}{2\cos^2\theta_W} = g_{hhZZ}^{SM} c_{2\theta} \,, \tag{3.32}$$

$$g_{\eta\eta WW} = -\frac{1}{4} g^2 s_\theta^2 \,, \tag{3.33}$$

$$g_{\eta\eta ZZ} = \frac{g_{\eta\eta WW}}{2\cos^2\theta_W} \,. \tag{3.34}$$

It can be seen that for $\theta \sim 0$ the couplings of h to W and Z are very similar to the ones of the Standard Model Higgs, while the couplings of η are suppressed by a factor s_θ^2. Moreover, if $\theta \sim 0$, the scale hierarchy $f \gg m_W$ is realised, according to which the TC-hadron masses are expected to be much larger than the electroweak scale. This is the limit in which the composite Goldstone Higgs scenario is realised. If θ is significantly larger than zero, the h particle stops looking similar to the Higgs, and the Higgs role is assumed by the lightest scalar resonance of the TC sector, as in Technicolor. If $\theta = \pi/2$, the two scalar particles h and η become degenerate (their couplings to W and Z are equal), and the associated complex state is stable and can play a role as dark matter candidate [15].

Unless flavour symmetry is explicitly broken, all the possible alignments of Σ_0 are equivalent. The introduction of electroweak interactions via partial gauging of SU(4) results in the explicit breaking of flavour symmetry. Gauge boson loops induce a potential for the Goldstone bosons, which is minimised by a specific value of the alignment angle θ. Moreover, also other possible symmetry-breaking contributions, such as interactions with SM fermions and mass terms for the TC-fermions, contribute to the potential, and influence the alignment of Σ_0. It is shown in [15] that the contribution of gauge boson loops to the one-loop potential contains mass terms for h and η, and is minimised at $\theta = 0$, corresponding to preserved electroweak symmetry.

A complete model of composite Higgs will contain some extra interactions on top of the ones mentioned until now, which are meant to generate masses for the SM fermions. For example, concentrating on the top quark mass, one could add to the Lagrangian 3.10 an effective four-fermion operator of the form:

$$\frac{y_t}{\Lambda_t^2}\bar{q}_L t_R \bar{u}_R Q_L + \text{h.c.}\,, \tag{3.35}$$

where q_L is the left-handed doublet containing the SM top and bottom quarks, $q_L = (t_L\, b_L)^T$, and t_R is the right-handed top quark. u_R and $Q_L = (u_L\, d_L)^T$ are TC-fermion fields. This is just an effective operator, which indicates that the theory should be extended by including some new interactions at energies larger than Λ_t. The contribution of this operator to the one-loop potential is minimised at $\theta = \pi/2$, i.e the Technicolor-like alignment [15].

The last source for the Goldstone boson potential analysed in [15] is a mass term for the TC-fermions. This term is assumed to be symmetric under $\mathrm{SU}(2)_L \times \mathrm{U}(1)_Y$, and therefore proportional to Σ_B: $M = \mu\Sigma_B$. It is found that, at the price of some fine tuning between the contributions of the top loop and the TC-fermion mass term, a small value of θ can be obtained, thus realising the composite Goldstone Higgs scenario.

The construction made until now is based on the assumption that the spontaneous symmetry breaking pattern $\mathrm{SU}(4) \to \mathrm{Sp}(4)$ is realised in the TC sector in isolation. This assumption must be verified via lattice simulations. Lattice studies of the SU(2) gauge theory with two fundamental fermions have found clear signs of symmetry breaking [16]: Goldstone boson states have been observed whose mass vanishes in the limit of vanishing fermion mass while the associated decay constant remains finite. Moreover, lattice simulations are the only way for measuring the mass spectrum of the theory, indicating in which energy range new particles are to be expected. In the case of the SU(2) model with two fundamental fermions, the lightest resonances have been found to lie beyond the present LHC limits, even in the Technicolor limit $\theta = \pi/2$ [16].

3.1.4 Fermion masses and partial compositeness

The setup of composite Higgs models must be extended in order to include massive fermion states. This is usually done by introducing in the Lagrangian operators which couple the SM fermions to the TC-fermions. The couplings can involve SM fermion bilinears, as in extended Technicolor [17, 18]:

$$\frac{\lambda_t}{\Lambda_{UV}^{d-1}}\bar{q}_L \mathcal{O} t_R + \text{h.c.}\,, \tag{3.36}$$

or can be linear in the SM fermions, as in partial compositeness [19]:

$$\frac{\lambda_t}{\Lambda_{UV}^{d_L-5/2}}\bar{q}_L \mathcal{O}^L + \frac{\bar{\lambda}_t}{\Lambda_{UV}^{d_R-5/2}}\bar{t}_R \mathcal{O}^R + \text{h.c.}\,. \tag{3.37}$$

In the previous equations we only listed the operators participating in the generation of the top quark mass. $q_L = (t_L\, b_L)$ represents the SM third quark family left-handed doublet, t_R the right-handed top quark and $\mathcal{O}$, $\mathcal{O}^L$, $\mathcal{O}^R$ composite operators of the TC sector. Generally the operators of equations 3.36, 3.37 are non-renormalisable, and the theory must be extended with new interactions at energies larger than Λ_{UV}. The operators 3.36, 3.37 thus arise as low-energy effective operators, accompanied by a power of Λ_{UV} dictated by the scaling dimension of $\mathcal{O}$, $\mathcal{O}^L$, $\mathcal{O}^R$ (d, d_L, d_R). The particle content of the TC sector must be chosen in such a way that the composite operators can have the correct quantum numbers for coupling with SM fermions. In particular the operator $\mathcal{O}$ of equation 3.36 must have the same quantum numbers as the SM Higgs, while $\mathcal{O}^L$ and $\mathcal{O}^R$ of equation 3.37 must have spin 1/2 and, on top of the electroweak quantum numbers, must also carry $\mathrm{SU}(3)_C$ charge. This means that, in the partial compositeness setup, the $\mathrm{SU}(3)_C$ symmetry must be embedded in the TC-fermion flavour symmetry, in such a way that it is not broken by the TC-fermion condensate.

In the partial compositeness scenario, fermion masses are generated via mixing between SM fermions and fermionic composite states of the TC sector. We denote by $\Lambda_{TC} < \Lambda_{UV}$ the scale at which the TC gauge coupling becomes strong, and we consider the effective theory arising when the ultraviolet cutoff is fixed to Λ_{TC}. In the model considered in [19], the operators $\mathcal{O}^L$, $\mathcal{O}^R$ mediate the coupling of the top quark to the same fermionic resonance B. The interactions in the effective Lagrangian look like:

$$\mathcal{L}_{eff}^{int} = c\Lambda_{TC}\big(\lambda_t(\Lambda_{TC})\bar{t}_L B_R + \bar{\lambda}_t(\Lambda_{TC})\bar{t}_R B_L\big) - m_B \bar{B}_L B_R + \text{h.c.}\,, \tag{3.38}$$

where c is an unknown coefficient and $\lambda_t(\Lambda_{TC})$, $\bar{\lambda}_t(\Lambda_{TC})$ are the coefficients appearing in equation 3.37 evolved down to the scale Λ_{TC}. Under the assumption $(c\Lambda_{TC})^2\lambda_t(\Lambda_{TC})\bar{\lambda}_t(\Lambda_{TC})/m_B^2 \ll 1$, the mass matrix has one light eigenvalue with mass

$$m_t \sim \frac{\lambda_t(\Lambda_{TC})\bar{\lambda}_t(\Lambda_{TC})}{m_B}(c\Lambda_{TC})^2\,, \tag{3.39}$$

and one heavier eigenvalue with mass $\sim m_B$. The physical top quark is identified with the light eigenstate, which is a superposition of the SM top and a TC composite state. This is the reason for the name partial compositeness: physical states are superpositions of elementary and composite states. The model proposed in [19], when extended to three families of SM quarks and leptons, is able to generate a large hierarchy of masses among the three families, having the first and second families much lighter than the third, even though a very general flavour structure is assumed in the underlying microscopic theory.

In the context of partial compositeness, it is difficult to generate a realistic top quark mass, without at the same time introducing flavour changing neutral currents (FCNC) incompatible with experimental constraints. In fact, the microscopic interactions that generate the operators 3.37 in general generate also couplings among four SM fermions, which may lead to large FCNC. For this reason, it is desirable to have a large separation between the scale of the new microscopic interactions and the scale at which the TC interaction becomes strong ($\Lambda_{UV} \gg \Lambda_{TC}$), thus suppressing the contribution from unwanted FCNC. However, this constraint suppresses the value of the top mass as well. It is usually assumed that the TC sector is close to a fixed point at energies $\sim \Lambda_{UV}$, so that:

$$\frac{\lambda_t}{\Lambda_{UV}^{d_L-5/2}} = \frac{\lambda_t(\Lambda_{TC})}{\Lambda_{TC}^{d_L-5/2}} \,, \quad \frac{\bar{\lambda}_t}{\Lambda_{UV}^{d_R-5/2}} = \frac{\bar{\lambda}_t(\Lambda_{TC})}{\Lambda_{TC}^{d_R-5/2}} \,. \tag{3.40}$$

It follows that the couplings relevant for the generation of the top quark mass are suppressed by a power of $\Lambda_{TC}/\Lambda_{UV}$:

$$\lambda_t(\Lambda_{TC}) = \lambda_t \left(\frac{\Lambda_{TC}}{\Lambda_{UV}}\right)^{d_L-\frac{5}{2}} \,, \quad \bar{\lambda}_t(\Lambda_{TC}) = \bar{\lambda}_t \left(\frac{\Lambda_{TC}}{\Lambda_{UV}}\right)^{d_R-\frac{5}{2}} \,. \tag{3.41}$$

A large value of $\Lambda_{TC}/\Lambda_{UV}$ is needed to satisfy the constraints on FCNC, while a small value would be needed for predicting a realistic top mass.

One may still obtain results compatible with experiments if the scaling dimensions of $\mathcal{O}^L$ and $\mathcal{O}^R$ are such that $d_L, d_R \sim 5/2$. We consider for example a model in which the fermionic operators $\mathcal{O}^L$, $\mathcal{O}^R$ are given by the product of three TC-fermion fields. In this case:

$$d_L = \frac{9}{2} - \gamma_L \,, \quad d_R = \frac{9}{2} - \gamma_R \,, \tag{3.42}$$

where $\gamma_{L,R}$ are the anomalous dimensions. Large anomalous dimensions $\gamma_{L,R} \sim 2$ would make it possible to have a large top mass, and at the same time suppressed FCNC. In fact, operators containing four SM fermions, responsible for FCNC, are not expected to develop large anomalous dimensions, since SM fermions are not coloured under the TC gauge interaction [19].

Recent studies indicate that the required large anomalous dimensions are hard to achieve. In particular, in [20] the SU(3) gauge theory with fundamental fermions is considered. The number of fermions is chosen in such a way that the theory is inside the conformal window, i.e. it has a nontrivial infrared fixed point. It is observed that the anomalous dimension of baryonic operators remains small down to the lowest point in the conformal window that can be analysed in perturbation theory. For a more detailed discussion of the conformal window see section 4.1

3.1.5 Fundamental Partial Compositeness

In order to overcome the difficulties related to the generation of fermion masses in composite Higgs scenarios, models of fundamental partial compositeness have recently been introduced [4]. In these models, the TC sector contains as matter fields not only fermions but also scalars. The Lagrangian can be written schematically as follows:

$$\mathcal{L} = \mathcal{L}_{SM}^{H=0} + \mathcal{L}_{TC}^{kin} + \mathcal{L}_Y - V_S \,, \tag{3.43}$$

where $\mathcal{L}_{SM}^{H=0}$ is the SM Lagrangian without the Higgs sector, $\mathcal{L}_{TC}^{kin}$ is the kinetic Lagrangian of the TC sector, containing eventual mass terms of TC-fermions and TC-scalars, $\mathcal{L}_Y$ contains Yukawa interactions among SM fermions, TC-fermions and TC-scalars, and V_S is the TC-scalar quartic potential.

The interactions between SM fermions and TC-fermions are mediated by Yukawa couplings with TC-scalars. At energies lower than Λ_{TC}, interactions between SM fermions and composite fermionic states formed by one TC-fermion and one TC-scalar are thus generated, and SM fermion masses arise via the partial compositeness mechanism. The name "fundamental" is due to the fact that only renormalisable operators appear in the Lagrangian. The low-energy effective field theory arising from this setup has been studied in detail in [21]. The implications for flavour physics and the compatibility with precision measurements of a minimal realisation of this scenario, i.e. containing the minimal number of new elementary particles, have been analysed in [22].

One may argue that, due to the presence of elementary scalars, models of fundamental partial compositeness are affected by the naturalness and triviality problems in the same way as the SM. While it is true that the naturalness problem is reintroduced, the scalars of fundamental partial compositeness may be free from the triviality problem. In fact, an ultraviolet fixed point may be present in the flow of the scalar quartic couplings. We will discuss this point in more detail in section 3.2. Moreover, the constraint $d_{L,R} \sim 5/2$ on the scaling dimensions of the operators $\mathcal{O}^{L,R}$ of equation 3.37 seems to indicate that operators with the scaling dimension of elementary scalars $d \sim 1$ must be present in the TC sector, which should mediate Yukawa-like couplings between SM fermions and TC-fermions. Therefore one may expect any purely fermionic realisation of partial compositeness to look at the effective level as the model described here [4] . Another interesting feature of the fundamental partial compositeness setup is that a complete theory of flavour is realised in a relatively self-contained way. This scenario offers a complete alternative to the Higgs mechanism of the SM.

As in the case of ordinary composite Higgs models, the pattern of global symmetry breaking assumed for the TC sector in isolation must be verified via lattice simulations. Specifically, in the model described in [21], the symmetry breaking pattern in the fermion sector is assumed to be SU($2N_f$)$\rightarrow$Sp($2N_f$), where N_f is the number of Dirac TC-fermion fields. The enlarged flavour symmetry SU($2N_f$) can be defined due to the fact that the gauge group is chosen as having a pseudo-real fundamental representation. In realistic models of fundamental partial compositeness, featuring more than one TC-scalar field, also the scalar sector is characterised by a global flavour symmetry. In the model described in [21], the scalar flavour symmetry is assumed not to be spontaneously broken by the formation of a scalar condensate. This assumption should also be tested on the lattice. Lattice measurements of the Wilson coefficients determined by the strong dynamics would also be of great interest in the context of the low-energy effective theory [21]. With these motivations, we started a lattice study of the SU(2) gauge theory with two fundamental fermions and one fundamental scalar. While this is not a realistic TC sector for a fundamental partial compositeness model, which would require multiple scalar fields, it is a good setup for a preliminary analysis of the impact of scalar fields on the symmetry breaking pattern and on the spectrum of composite states.

3.2 Perturbative aspects of the continuum theory

The object of our lattice analysis is the SU(2) theory with two fundamental fermions and one fundamental scalar. Before entering in the details of the lattice study, we mention some interesting aspects of the continuum theory, related to the running of the scalar quartic couplings.

For these first considerations, we analyse a more general model, with SU(N) gauge group, and N_f fermions and N_S scalars in the fundamental representation. We organise the scalar and fermion fields into matrices carrying a colour index α and a flavour index i: $S_{\alpha i}$, $Q_{\alpha i}$, and we write the Lagrangian as:

$$\mathcal{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \mathrm{tr}\big[\bar{Q} i \not{D} Q\big] + \mathrm{tr}\big[(D_\mu S)^\dagger D^\mu S\big] - V_S \,, \tag{3.44}$$

where V_S is the scalar quartic potential. The most general quartic operators invariant under both SU(N) and a global SU(N_S) flavour symmetry are:

$$\big(\mathrm{tr}\big[S^\dagger S\big]\big)^2 = S^*_{i\alpha} S_{\alpha i} S^*_{j\beta} S_{\beta j} \,, \quad \mathrm{tr}\big[S^\dagger S S^\dagger S\big] = S^*_{i\alpha} S_{\alpha j} S^*_{j\beta} S_{\beta i} \,. \tag{3.45}$$

It follows that the scalar quartic potential, respecting colour and flavour symmetries, is given by:

$$V_S = \lambda_1 \big(\mathrm{tr}\big[S^\dagger S\big]\big)^2 + \lambda_2 \, \mathrm{tr}\big[S^\dagger S S^\dagger S\big] \,. \tag{3.46}$$

If $N_S = 1$, the two operators of equation 3.45 are equal, and one single scalar quartic coupling $\lambda = \lambda_1 + \lambda_2$ is present in the Lagrangian. Since it is of interest for the model studied in this thesis, we specialise the following considerations to the case $N_S = 1$. A complete analysis with generic N_S has been carried out in [23].

The one-loop beta functions of the gauge coupling g and the scalar quartic coupling λ are given by [4]:

$$\begin{aligned} (4\pi)^2 \beta_g &= -\left(\frac{11}{3}N - \frac{2}{3}N_f - \frac{1}{6}\right) g^3 \,, \\ (4\pi)^2 \beta_\lambda &= 4(N+4)\lambda^2 - \frac{6(N^2-1)}{N} g^2 \lambda + \frac{3N^3 + 3N^2 - 12N + 6}{4N^2} g^4 \,. \end{aligned} \tag{3.47}$$

The running of g and λ as functions of the energy scale μ is determined by solving the renormalisation group equations:

$$\frac{\mathrm{d}g}{\mathrm{d}\ln\mu} = \beta_g(g) \,, \quad \frac{\mathrm{d}\lambda}{\mathrm{d}\ln\mu} = \beta_\lambda(\lambda, g) \,. \tag{3.48}$$

Depending on the choice of N and N_f, the solutions may display complete asymptotic freedom, i.e. both g and λ go to zero in the limit of large μ. In this case the theory is well defined at high energies and does not suffer from the triviality problem, even though it contains elementary scalars. As an example, we report in figure 3.1 the running of g^2 and λ in the case $N = 5$, $N_f = 26$. It can be seen that, while g^2 always goes to zero at high energies, the initial condition of λ can be chosen such that also λ flows to zero, thus realising complete asymptotic freedom. In table 3.1 we report, for different values of N, the ranges in N_f such that there exist completely asymptotically free solutions. It can be noticed that for $N = 2$, the object of our lattice study, there is no possible choice of N_f leading to complete asymptotic freedom. Nevertheless the case $N = 2$ is of great interest. In fact, as shown in section 3.1.3, the SU(2) gauge theory with two fundamental fermions offers a minimal setup for composite Higgs models, and for this reason it has been extensively studied on the lattice [16]. Adding a fundamental scalar to this setup seems to be the first mandatory step to be taken, in order to observe the impact of TC-scalars on the dynamics of the TC sector in a fundamental partial compositeness scenario.

Figure 3.2 shows the running of g^2 and λ in the SU(2) gauge theory with two fundamental fermions and one fundamental scalar. Two different initial conditions are chosen for λ: $\lambda_0 = \lambda(\mu_0) = 0$, and $\lambda_0 = \lambda(\mu_0) = 0.2$. While in both cases the coupling λ diverges at high energies, this happens at an energy scale which is very large compared to the scale at which $g^2 = 1$. Specifically, if we assume that $g^2 = 1$ at $\mu_0 \sim 10^3$ GeV, then the singularity is located beyond the Planck scale ($\ln(\mu_{Pl}/\mu_0) \sim 37$) for both choices of initial conditions.

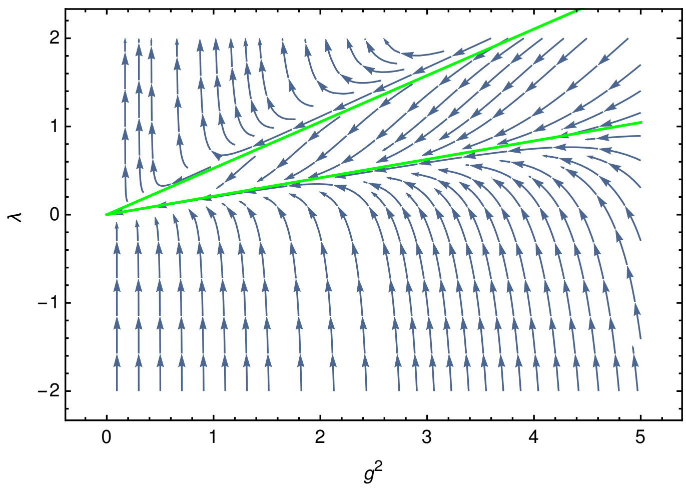

Figure 3.1: Running of the squared gauge coupling g^2 and of the scalar quartic coupling λ for a theory with SU(5) gauge group, $N_f = 26$ fundamental fermions and $N_S = 1$ fundamental scalars. The arrows indicate the direction of increasing energy. The green lines represent the fixed flow solutions of the renormalisation group equations, characterised by a constant ratio λ/g^2.

One more comment must be made regarding the case $N = 2$. As previously pointed out, the fundamental representation of SU(2) is pseudo-real. One may wonder whether in this case there exist more quartic operators than the ones listed in equation 3.45. It is shown in appendix A.4 that, also in the case of an SU(2) gauge group, the most general quartic potential takes the form 3.46.

3.3 Lattice setup

We now move to the lattice study of the SU(2) gauge theory with two fundamental fermions and one fundamental scalar. In section 3.2, we discussed the running

Table 3.1: For different values of N, ranges in N_f such that there exist completely asymptotically free solutions, in a theory with SU(N) gauge group, N_f fundamental fermions and $N_S = 1$ fundamental scalars.

N	N_f
2	No solutions
3	$15.93 < N_f < 16.25$
4	$19.8 < N_f < 21.75$
5	$23.56 < N_f < 27.25$
6	$27.27 < N_f < 32.75$
7	$30.94 < N_f < 38.25$
8	$34.6 < N_f < 43.75$
9	$38.24 < N_f < 49.25$
10	$41.88 < N_f < 54.75$

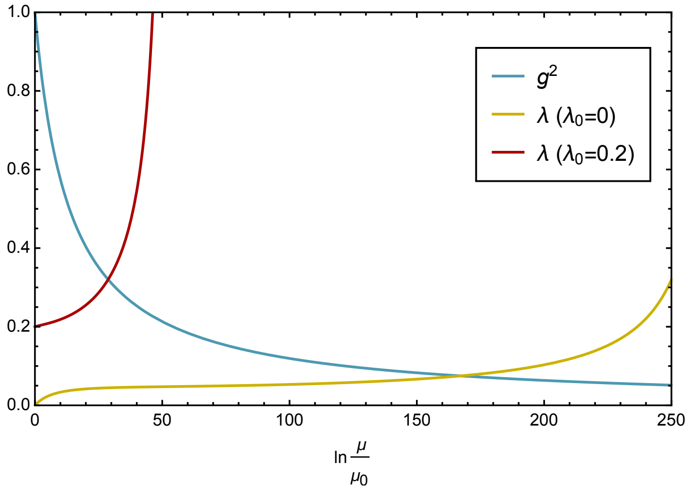

Figure 3.2: Running of g^2 and λ as functions of $\ln(\mu/\mu_0)$ in an SU(2) gauge theory with $N_f = 2$ fundamental fermions and $N_S = 1$ fundamental scalars. λ is plotted for two different initial conditions: $\lambda_0 = \lambda(\mu_0) = 0$, and $\lambda_0 = \lambda(\mu_0) = 0.2$.

of the scalar quartic coupling, and we concluded that the SU(2) theory is not well defined at high energies because the quartic coupling diverges. Because of this, it is impossible to define the continuum limit of the lattice theory. In fact, due to the universality of the first two coefficients of the beta function, the running of the lattice bare couplings as functions of the lattice spacing is the same as shown in figure 3.2, with $\mu \propto 1/a$. It follows that, at least in the region where perturbation theory is valid, there is no critical point in the space of bare lattice parameters, and the program of taking the lattice spacing to zero while moving on lines of constant physics cannot be undertaken. Instead, one can take the lattice spacing down to some small but finite value, and match the lattice theory to an effective theory with an ultraviolet cutoff. Given the running of the scalar quartic coupling shown in figure 3.2, we expect the lattice theory to present a good scaling window when changing the lattice spacing, so that valuable input for phenomenological models can be provided.

For our lattice study, we generated gauge and scalar field configurations with the HiRep code, first introduced in [24], which we extended in order to simulate the scalar field in addition to gauge and fermions. In the following we describe the lattice action and the resulting forces needed for the implementation of the Hybrid Monte Carlo algorithm.

3.3.1 Action

For the gauge and fermion action we use the Wilson discretisation, as defined in equation 2.53. For simplicity, we fix the lattice spacing to one, and we use the standard notation $\beta = 2N/g^2 = 4/g^2$. As for the scalar field S, we consider the Euclidean continuum action:

$$S_S^{cont}[A, S^\dagger, S] = \int d^4x \Big((D_\mu S)^\dagger D_\mu S + m_S^2 |S|^2 + \lambda |S|^4 \Big) , \tag{3.49}$$

and we discretise it by assigning

$$\int \mathrm{d}^4 x (D_\mu S)^\dagger D_\mu S \to -\sum_{x,\mu} S^\dagger \nabla_\mu^* \nabla_\mu S , \tag{3.50}$$

where

$$\begin{aligned} \nabla_\mu S(x) &= U_\mu(x) S(x+\hat{\mu}) - S(x) \\ \nabla_\mu^* S(x) &= S(x) - U_\mu(x-\hat{\mu})^\dagger S(x-\hat{\mu}) . \end{aligned} \tag{3.51}$$

The resulting discretised action is:

$$\begin{aligned} S_S[U, S^\dagger, S] = &\sum_x \Bigg[-\sum_\mu \Big(S^\dagger(x) U_\mu(x) S(x+\hat{\mu}) + S^\dagger(x) U_\mu(x-\hat{\mu})^\dagger S(x-\hat{\mu}) \Big) + \\ & M^2 S^\dagger(x) S(x) + \lambda \big(S^\dagger(x) S(x) \big)^2 \Bigg] , \end{aligned} \tag{3.52}$$

where $M^2 = m_S^2 + 8$. For future purposes, we write the action of our lattice model as:

$$S[U, \phi^\dagger, \phi, S^\dagger, S] = S_G[U] + S_F[U, \phi^\dagger, \phi] + S_S[U, S^\dagger, S] , \tag{3.53}$$

where S_S is the scalar contribution given by equation 3.52, S_G is the gauge contribution:

$$S_G[U] = \beta \sum_{x \in \Lambda} \sum_{\mu < \nu} \left[1 - \frac{1}{\mathrm{N}} \mathrm{Re}\,\mathrm{tr}[U_{\mu\nu}] \right] , \tag{3.54}$$

and S_F the pseudofermion contribution:

$$S_F[U, \phi^\dagger, \phi] = \sum_{x,y \in \Lambda} \phi^\dagger(x) Q^{-2}(x|y) \phi(y) \equiv \phi^\dagger Q^{-2} \phi , \tag{3.55}$$

where we introduced a short-hand notation that will be useful in the following.

3.3.2 Forces

In order to implement the Hybrid Monte Carlo algorithm, we introduce the Hamiltonian:

$$H = \frac{1}{2} T_R \sum_{x,\mu} \sum_{a=1}^{N^2-1} \pi_a(x,\mu)^2 + \sum_x \sum_{i=1}^{N} P_i(x) P_i^*(x) + S[U, \phi^\dagger, \phi, S^\dagger, S] \,, \qquad (3.56)$$

where $\pi_a(x,\mu)$ and $P_i(x)$ are the momenta associated to the gauge and scalar fields, and S is the action 3.53. Here, to be more general, we are referring to an SU(N) gauge group. T_R is the normalisation of the SU(N) generators in the representation R, defined by: $\mathrm{tr}(T^a T^b) = T_R \delta^{ab}$. In this setup, only gauge and scalar fields evolve dynamically along the molecular dynamics trajectory. The pseudofermions are updated before starting every new trajectory according to the following rule: a field χ is extracted out of a Gaussian distribution, with probability $P[\chi] \propto \exp\left[-\chi^\dagger \chi\right]$, and then the pseudofermion field is defined as: $\phi = D\chi$, where D is the Wilson-Dirac operator 2.46. The field ϕ defined in this way is correctly distributed according to:

$$\det\left[Q^2\right] = \det[D]^2 = \det\left[DD^\dagger\right] = \pi^{-N} \int \prod_{x \in \Lambda} \mathrm{d}\phi(x) \mathrm{d}\phi^\dagger(x) \exp\left[-\phi^\dagger (DD^\dagger)^{-1} \phi\right] . \qquad (3.57)$$

We express the link variables as:

$$U_\mu(x) = \exp\left[\frac{i}{T_R} q_a(x,\mu) T^a\right] , \qquad (3.58)$$

and we assign the conjugate momenta as follows:

$$\begin{aligned} &q_a(x,\mu) \to \pi_a(x,\mu) \\ &S_i(x) \to P_i(x) \, . \end{aligned} \qquad (3.59)$$

Hamilton's equations are given by:

$$\begin{aligned} \dot{q}_a(x,\mu) &= \frac{\partial H}{\partial \pi_a(x,\mu)} = T_R \pi_a(x,\mu) \\ \dot{\pi}_a(x,\mu) &= -\frac{\partial H}{\partial q_a(x,\mu)} = -\frac{\partial S_G}{\partial q_a(x,\mu)} - \frac{\partial S_F}{\partial q_a(x,\mu)} - \frac{\partial S_S}{\partial q_a(x,\mu)} \\ \dot{S}_i(x) &= \frac{\partial H}{\partial P_i(x)} = P_i^*(x) \\ \dot{P}_i(x) &= -\frac{\partial H}{\partial S_i(x)} = -\frac{\partial S_S}{\partial S_i(x)} \, , \end{aligned} \qquad (3.60)$$

where the dot indicates the derivative with respect to molecular dynamics time. For brevity we omitted the equations for $\dot{S}^*$ and $\dot{P}^*$, which are simply given by the complex conjugate of the last two lines in 3.60. The first line of 3.60 can be rewritten in terms of the link variables as follows:

$$\dot{U}_\mu(x) = i\pi_a(x,\mu)T^a U_\mu(x) \ . \tag{3.61}$$

The driving forces are given by:

- $$\frac{\partial S_G}{\partial q_a(x,\mu)} = -\frac{\beta}{N}\frac{1}{T_R}\mathrm{Re}\ \mathrm{tr}\left[iT^a U_\mu(x)V_\mu^\dagger(x)\right] \tag{3.62}$$

where $V_\mu(x) = \sum_{\nu\neq\mu}\left[U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\hat{\mu}) + U_\nu^\dagger(x-\hat{\nu})U_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu}+\hat{\mu})\right]$ is the sum of the staples around the link $U_\mu(x)$,

- $$\frac{\partial S_F}{\partial q_a(x,\mu)} = -\left[\phi^\dagger Q^{-2}\frac{\partial Q}{\partial q_a(x,\mu)}Q^{-1}\phi + \phi^\dagger Q^{-1}\frac{\partial Q}{\partial q_a(x,\mu)}Q^{-2}\phi\right] \tag{3.63}$$

where

$$\frac{\partial Q(x|y)}{\partial q_a(z,\mu)} = \gamma_5\left(-\frac{i}{2T_R}(\mathbb{1}-\gamma_\mu)T^a U_\mu(z)\delta_{y,z+\hat{\mu}}\delta_{x,z} + \frac{i}{2T_R}(\mathbb{1}+\gamma_\mu)U_\mu^\dagger(z)T^a\delta_{y,z}\delta_{x-a\hat{\mu},z}\right), \tag{3.64}$$

- $$\frac{\partial S_S}{\partial q_a(x,\mu)} = -\frac{2}{T_R}\ \mathrm{Re}\left[S^\dagger(x)iT^a U_\mu(x)S(x+\hat{\mu})\right] \tag{3.65}$$

- $$\begin{aligned}\frac{\partial S_S}{\partial S_i(x)} = &-\sum_\mu\left(S_k^*(x-\hat{\mu})U_\mu(x-\hat{\mu})_{ki} + S_k^*(x+\hat{\mu})U_\mu(x)_{ki}^\dagger\right) + \\ &+ M^2 S_i^*(x) + 2\lambda S_k^*(x)S_k(x)S_i^*(x) \ .\end{aligned} \tag{3.66}$$

Hamilton's equations 3.60 are to be solved numerically, thus generating the molecular dynamics trajectory. In this work we used a second-order Omelyan integrator [25, 26] for the numerical integration.

3.4 Spectrum

3.4.1 Mesons

Finite volume corrections + dependence on m_{PCAC}

3.4.2 Scalar-scalar states

3.4.3 Fermion-scalar states

3.5 Phase space

3.5.1 Phase diagram of the SU(2)-Higgs model

3.5.2 Gauge fixing

3.5.3 Results

3.6 Conclusions and outlook

Chapter 4

Transport coefficients in the conformal window

4.1 The conformal window

4.2 Transport coefficients

4.3 Transport coefficients in a quantum field theory

4.4 Application of perturbative results to theories in the conformal window

Chapter 5

Conclusions

Appendix A

A.1 General conventions and definitions

In this appendix we introduce the general notations and conventions used in the thesis.

A.1.1 Metric and units

We use the following convention for Minkowski metric:

$$(\eta_{\mu\nu}) = \mathrm{diag}[1, -1, -1, -1]\,. \tag{A.1}$$

As for the unit system, we use natural units, where both the speed of light c and the reduced Planck constant $\hbar$ are set equal to one.

A.1.2 Gamma matrices

Gamma matrices appear in the Dirac Lagrangian: $\mathcal{L}_D[\bar{\psi}, \psi] = \bar{\psi}(i\gamma^\mu D_\mu - m\mathbb{1})\psi$, and fulfil the following relations:

- Clifford algebra: $\{\gamma^\mu, \gamma^\nu\} = 2\mathbb{1}\eta^{\mu\nu}$
- Relation with the hermitian conjugate: $\gamma^\mu = \gamma^0(\gamma^\mu)^\dagger\gamma^0 \quad .$

As a consequence, the following equations hold:

- $(\gamma^0)^2 = \mathbb{1}$, $(\gamma^i)^2 = -\mathbb{1}$, $i = 1, 2, 3$
- $(\gamma^0)^\dagger = \gamma^0$, $(\gamma^i)^\dagger = -\gamma^i$, $i = 1, 2, 3$
- $\{\gamma^\mu, \gamma^\nu\} = 0$ if $\mu \neq \nu \quad .$

γ_5 is defined by: $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$, and it has the following properties: $(\gamma_5)^2 = \mathbb{1}$, $(\gamma_5)^\dagger = \gamma_5$, $\{\gamma_5, \gamma^\mu\} = 0$. There exist multiple representations of the gamma matrices, and physical results do not depend on the choice of the representation. In this thesis we use the chiral representation:

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1}_{2\times2} \\ \mathbb{1}_{2\times2} & 0 \end{pmatrix}\,, \qquad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}\,, \qquad \gamma_5 = \begin{pmatrix} -\mathbb{1}_{2\times2} & 0 \\ 0 & \mathbb{1}_{2\times2} \end{pmatrix}\,, \tag{A.2}$$

where σ^i, $i = 1, 2, 3$, are the Pauli matrices.

Gamma matrices are involved in the definition of the Lorentz group representation acting on Dirac spinors. In particular, the generators of Lorentz transformations are defined by: $J^{\mu\nu} = -i/4[\gamma^\mu, \gamma^\nu]$. Moreover, the parity transformation of a Dirac spinor is defined by:

$$\psi(\mathbf{x}, t) \to \psi'(\mathbf{x}, t) = \gamma^0 \psi(-\mathbf{x}, t) \,, \tag{A.3}$$

and the transformation under charge conjugation by:

$$\psi(x) \to \psi^C(x) = C\bar{\psi}(x)^T \,, \tag{A.4}$$

where the charge conjugation operator is $C = i\gamma^2\gamma^0$.

γ_5 appears in the definition of the chirality projectors:

$$P_L = \frac{\mathbb{1} - \gamma_5}{2} \,, \qquad P_R = \frac{\mathbb{1} + \gamma_5}{2} \,, \tag{A.5}$$

which have the following properties: $P_{R,L}^2 = P_{R,L}$, $P_R P_L = P_L P_R = 0$, $P_L + P_R = \mathbb{1}$, and are used to define left- and right-handed spinors:

$$\psi(x) = \psi_L(x) + \psi_R(x) \,, \qquad \psi_L(x) = P_L\psi(x) \,, \qquad \psi_R(x) = P_R\psi(x) \,. \tag{A.6}$$

The Dirac Lagrangian can be rewritten in terms of left- and right-handed Dirac spinors as follows:

$$\mathcal{L}_D = \bar{\psi}_L(i\gamma^\mu D_\mu)\psi_L + \bar{\psi}_R(i\gamma^\mu D_\mu)\psi_R - m(\bar{\psi}_L\psi_R + \bar{\psi}_R\psi_L) \,. \tag{A.7}$$

The Dirac Lagrangian in Euclidean space is: $\mathcal{L}_D^E[\bar{\psi}, \psi] = \bar{\psi}(\gamma_\mu^E D_\mu + m\mathbb{1})\psi$, where the relation between Minkowskian and Euclidean gamma matrices is:

$$\gamma_0^E = \gamma_0 \,, \qquad \gamma_i^E = i\gamma_i = -i\gamma^i \,. \tag{A.8}$$

Euclidean gamma matrices have the following properties:

- $\left\{\gamma_\mu^E, \gamma_\nu^E\right\} = 2\mathbb{1}\delta_{\mu\nu} \Rightarrow (\gamma_\mu^E)^2 = \mathbb{1}$
- $(\gamma_\mu^E)^\dagger = \gamma_\mu^E$

Euclidean γ_5 is defined by: $\gamma_5^E = \gamma_1^E\gamma_2^E\gamma_3^E\gamma_0^E$, and has analogue properties to Minkowskian γ_5: $(\gamma_5^E)^2 = \mathbb{1}$, $(\gamma_5^E)^\dagger = \gamma_5^E$, $\left\{\gamma_5^E, \gamma_\mu^E\right\} = 0$.

Euclidean gamma matrices in the chiral representation are given by:

$$\gamma_0^E = \begin{pmatrix} 0 & \mathbb{1}_{2\times2} \\ \mathbb{1}_{2\times2} & 0 \end{pmatrix} \,, \qquad \gamma_i^E = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix} \,, \qquad \gamma_5^E = \begin{pmatrix} \mathbb{1}_{2\times2} & 0 \\ 0 & -\mathbb{1}_{2\times2} \end{pmatrix} \,. \tag{A.9}$$

In this thesis we always omit the superscript E in gamma matrices, and we implicitly assume that every time we discuss a lattice model, which requires the Euclidean version of the action, gamma matrices assume their Euclidean form.

A.1.3 Algebra of SU(N) generators

A.2 Lattice Fourier transforms

In this appendix we define Fourier transforms on the lattice. The lattice Λ is defined as:

$$\Lambda = \{ x_\mu = n_\mu a \mid n_\mu = 0, \dots, L_\mu - 1,\ \mu = 0, \dots, 3 \} \ , \tag{A.10}$$

where a is the lattice spacing and L_μ the number of lattice points in direction μ. The total number of lattice points V is given by: $V = \prod_{\mu=0}^{3} L_\mu$.

We consider a function $f(x)$ defined on the lattice, and we define its Fourier transform as:

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{V}} \sum_{p \in \tilde{\Lambda}} \tilde{f}(p) e^{ip\cdot x} \\ \tilde{f}(p) &= \frac{1}{\sqrt{V}} \sum_{x \in \Lambda} f(x) e^{-ip\cdot x} \end{aligned} \tag{A.11}$$

where $\tilde{\Lambda}$ denotes the momentum space. Since the space-time has a finite volume, the momenta belong to a discrete set. Specifically, if periodic boundary conditions are imposed in direction μ, i.e. $f(x + aL_\mu\hat{\mu}) = f(x)$, then p_μ takes values in the discrete set $\{ p_\mu = \frac{2\pi}{aL_\mu} k_\mu \mid k_\mu \in \mathbb{Z} \}$. While in the case of anti-periodic boundary conditions, $f(x + aL_\mu\hat{\mu}) = -f(x)$, p_μ belongs to $\{ p_\mu = \frac{2\pi}{aL_\mu}(\frac{1}{2} + k_\mu) \mid k_\mu \in \mathbb{Z} \}$. Moreover, since the coordinates x_μ of each lattice point are represented by integer numbers of lattice spacings, the momenta are periodic: $\tilde{f}(p) = \tilde{f}(p + \frac{2\pi}{a}\hat{\mu})$. Therefore, the momentum space is defined as:

$$\tilde{\Lambda} = \{ p_\mu = \frac{2\pi}{aL_\mu}(k_\mu + \theta_\mu) \mid k_\mu = -\frac{L_\mu}{2} + 1, \dots, \frac{L_\mu}{2},\ \mu = 0, \dots, 3 \} \ , \tag{A.12}$$

where $\theta_\mu = 0$ corresponds to periodic boundary conditions in direction μ, and $\theta_\mu = 1/2$ to anti-periodic ones.

The lattice delta functions are defined as:

$$\begin{aligned} \delta(x - x') &= \delta_{n_0,n_0'}\delta_{n_1,n_1'}\delta_{n_2,n_2'}\delta_{n_3,n_3'} = \frac{1}{V} \sum_{p \in \tilde{\Lambda}} e^{ip\cdot(x-x')} \\ \delta(p - p') &= \delta_{k_0,k_0'}\delta_{k_1,k_1'}\delta_{k_2,k_2'}\delta_{k_3,k_3'} = \frac{1}{V} \sum_{x \in \Lambda} e^{i(p-p')\cdot x} \ . \end{aligned} \tag{A.13}$$

A.3 Hybrid Monte Carlo and the detailed balance relation

In this appendix we show that the HMC algorithm respects the detailed balance relation 2.15. We consider a scalar field theory with action $S[\phi]$. According to equation 2.54, the expectation value of an observable O is given by:

$$\langle O \rangle = \frac{\int \prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x)\, O[\phi] e^{-H[\pi,\phi]}}{\int \prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x)\, e^{-H[\pi,\phi]}} , \tag{A.14}$$

where the Hamiltonian is defined by: $H[\pi, \phi] = \frac{1}{2}\sum_x \pi(x)^2 + S[\phi]$.

The HMC algorithm consists of the following steps:

- The momenta $\pi(x)$ are extracted from a Gaussian distribution, with probability $P[\pi(x)] \propto \exp[-\pi(x)^2/2]$. This way an initial configuration of the momenta is defined

- Starting from the initial configuration (π, ϕ), the system evolves to a new state (π', ϕ') along a molecular dynamics trajectory which is a numerical solution of Hamilton's equations 2.55

- The final configuration (π', ϕ') is accepted or rejected in a Metropolis step, according to the transition probability

$$W_M(\pi, \phi \to \pi'\phi') = \min\left[1, \frac{e^{-H[\pi',\phi']}}{e^{-H[\pi,\phi]}}\right] . \tag{A.15}$$

We denote by $W_{\mathrm{md}}(\pi, \phi \to \pi', \phi')$ the probability of evolving from the state (π, ϕ) to (π', ϕ') along the molecular dynamics trajectory. We stress however that molecular dynamics is a deterministic process, and, given an initial state, all the following states in the trajectory are uniquely determined.

We further assume that the numerical integrator generating the molecular dynamics trajectory fulfils the following conditions:

- Preservation of the integration measure: $\prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x) = \prod_x \mathrm{d}\phi'(x)\mathrm{d}\pi'(x)$

- Reversibility: $W_{\mathrm{md}}(\pi, \phi \to \pi', \phi') = W_{\mathrm{md}}(-\pi', \phi' \to -\pi, \phi)$.

The probability to evolve from a scalar field configuration ϕ to ϕ' in one HMC step is given by:

$$W(\phi \to \phi') = \int \prod_x \mathrm{d}\pi(x)\mathrm{d}\pi'(x) W_M(\pi, \phi \to \pi', \phi') W_{\mathrm{md}}(\pi, \phi \to \pi', \phi') e^{-\sum_x \pi(x)^2/2} . \tag{A.16}$$

We rewrite Metropolis transition probability as follows:

$$\begin{aligned} W_M(\pi, \phi \to \pi', \phi') &= \min\left[1, \frac{e^{-H[\pi',\phi']}}{e^{-H[\pi,\phi]}}\right] = \frac{e^{-H[\pi',\phi']}}{e^{-H[\pi,\phi]}} \min\left[1, \frac{e^{-H[\pi,\phi]}}{e^{-H[\pi',\phi']}}\right] = \\ &= \exp\left[-\frac{1}{2}\sum_x \pi'(x)^2 - S[\phi'] + \frac{1}{2}\sum_x \pi(x)^2 + S[\phi]\right] W_M(\pi', \phi' \to \pi, \phi) , \end{aligned} \tag{A.17}$$

and we insert this expression in equation A.33:

$$W(\phi \to \phi') = \int \prod_x \mathrm{d}\pi(x)\mathrm{d}\pi'(x) W_M(\pi', \phi' \to \pi, \phi) W_{\mathrm{md}}(\pi, \phi \to \pi', \phi') \times \\ \exp\Bigg[-\frac{1}{2}\sum_x \pi'(x)^2 - S[\phi'] + S[\phi]\Bigg] . \tag{A.18}$$

We now use the reversibility of the molecular dynamics trajectory, together with the fact that $W_M(\pi, \phi \to \pi', \phi')$ is quadratic in π and π':

$$\begin{aligned} W(\phi \to \phi') =& \exp\big[-S[\phi'] + S[\phi]\big] \int \prod_x \mathrm{d}\pi(x)\mathrm{d}\pi'(x) W_M(-\pi', \phi' \to -\pi, \phi) \times \\ & W_{\mathrm{md}}(-\pi', \phi' \to -\pi, \phi) \exp\big[-\sum_x \pi'(x)^2/2\big] = \\ =& \exp\big[-S[\phi'] + S[\phi]\big] W(\phi' \to \phi) , \end{aligned} \tag{A.19}$$

where in the last step we used the fact that the integration measure $\int \prod_x \mathrm{d}\pi(x)\mathrm{d}\pi'(x)$ and the factor $\exp\big[-\sum_x \pi'(x)^2/2\big]$ are invariant under a change of sign of π and π'. The detailed balance relation follows directly from equation A.34:

$$\exp\big[-S[\phi]\big] W(\phi \to \phi') = \exp\big[-S[\phi']\big] W(\phi' \to \phi) . \tag{A.20}$$

In the above proof we used explicitly the reversibility of the molecular dynamics process. The preservation of the integration measure $\prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x) = \prod_x \mathrm{d}\phi'(x)\mathrm{d}\pi'(x)$ is also required, because it ensures that in the path integral $\int \prod_x \mathrm{d}\phi(x)\mathrm{d}\pi(x) e^{-H[\pi,\phi]}$ each configuration is actually weighted by $e^{-H[\pi,\phi]}$, without the appearance of an extra Jacobian determinant. (?????????????????????????????)

A.4 Scalar quartic potential in an SU(2) gauge theory

We consider a theory of gauge-interacting scalars in the fundamental representation of the gauge group SU(2). We discuss which terms are allowed by colour and flavour symmetries in the quartic potential.

A.4.1 Single scalar field

We first consider the case of one single scalar field ϕ. A gauge transformation is given by:

$$\phi \to \phi' = U\phi \tag{A.21}$$

where $U \in$ SU(2)=Sp(2) is characterised by:

$$\begin{cases} U^\dagger U = \mathbb{1} \\ U^T \epsilon U = \epsilon \end{cases} , \tag{A.22}$$

ϵ being the two-dimensional antisymmetric tensor:

$$\epsilon = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{A.23}$$

We can construct a field $\tilde{\phi} = -\epsilon\phi^*$ which transforms in the same way as ϕ under a gauge transformation: $\tilde{\phi} \to \tilde{\phi}' = U\tilde{\phi}$. We define a matrix S

$$S = (\phi, \tilde{\phi}) \tag{A.24}$$

which transforms as: $S \to S' = US$. The relation $\tilde{\phi} = -\epsilon\phi^*$ is translated in a relation between S and S^*:

$$S^* = -\epsilon S E \, , \tag{A.25}$$

where

$$E = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} . \tag{A.26}$$

Eq. A.25 can be verified as follows: we write the entries of S as S_{ia}, where $i = 1, 2$ is the colour index and $a = 1, 2$ is the flavour index, then we have $S_{i1} = \phi_i$, $S_{i2} = -\epsilon_{ij}\phi_j^* = -\epsilon_{ij}S_{j1}^*$. It follows that:

$$\begin{array}{l} (\epsilon SE)_{i1} = \epsilon_{ij}S_{ja}E_{a1} = -\epsilon_{ij}S_{j2} = -\epsilon_{ij}(-\epsilon_{jk}S_{k1}^*) = -\delta_{ik}S_{k1}^* = -S_{i1}^* \\ (\epsilon SE)_{i2} = \epsilon_{ij}S_{ja}E_{a2} = \epsilon_{ij}S_{j1} = -S_{i2}^* \end{array} . \tag{A.27}$$

The kinetic term of the scalar Lagrangian is expressed in terms of S as follows:

$$\mathcal{L}_{kin} = \frac{1}{2}\mathrm{Tr}\big[(D_\mu S)^\dagger (D^\mu S)\big] . \tag{A.28}$$

Given a matrix $M \in \mathrm{U}(2)$ we define a flavour transformation

$$S \to S' = SM \, , \tag{A.29}$$

and we work out the conditions under which it is a symmetry of the kinetic term A.28. If we require $S'^* = -\epsilon S' E$, it follows that M must fulfil the following constraint:

$$EM^* = ME \, , \tag{A.30}$$

which, together with the fact that M is a unitary matrix, implies:

$$E = MEM^T . \tag{A.31}$$

The flavour symmetry group is therefore Sp(2)=SU(2).

The possible terms which are quartic in the field ϕ and symmetric under colour and flavour transformations are the following:

$$
\begin{matrix}
\left(\mathrm{Tr}\left[S^\dagger S\right]\right)^2 \\
\mathrm{Tr}\left[S^\dagger S S^\dagger S\right] \\
\left(\mathrm{Tr}\left[S^T \epsilon S E\right]\right)^2 \\
\mathrm{Tr}\left[S^T \epsilon S E S^T \epsilon S E\right]
\end{matrix} . \tag{A.32}
$$

The last two terms in A.32 can be shown to be equal to the first ones by applying equation A.25:

$$
\begin{aligned}
\left(\mathrm{Tr}\left[S^T \epsilon S E\right]\right)^2 &= \left(\mathrm{Tr}\left[S^T(-S^*)\right]\right)^2 = \left(-\mathrm{Tr}\left[(S^\dagger S)^*\right]\right)^2 \\
&= \left(\mathrm{Tr}\left[(S^\dagger S)\right]\right)^2
\end{aligned} , \tag{A.33}
$$

$$
\begin{aligned}
\mathrm{Tr}\left[S^T \epsilon S E S^T \epsilon S E\right] &= \mathrm{Tr}\left[S^T(-S^*) S^T (-S^*)\right] = \mathrm{Tr}\left[(S^\dagger S)^* (S^\dagger S)^*)\right] \\
&= \mathrm{Tr}\left[S^\dagger S S^\dagger S\right] .
\end{aligned} \tag{A.34}
$$

The first and the second term in equation A.32 are not linearly independent when only one scalar field is present. To show this we start by explicitly writing $S^\dagger S$:

$$
\left.
\begin{aligned}
&S^\dagger S = \begin{pmatrix} \phi^\dagger \phi & \phi^\dagger \tilde{\phi} \\ \tilde{\phi}^\dagger \phi & \tilde{\phi}^\dagger \tilde{\phi} \end{pmatrix} \\
&\phi^\dagger \tilde{\phi} = -\phi_i^* \epsilon_{ij} \phi_j^* = 0 \\
&\tilde{\phi}^\dagger \phi = -\epsilon_{ij} \phi_j \phi_i = 0 \\
&\tilde{\phi}^\dagger \tilde{\phi} = -\epsilon_{ij} \phi_j (-\epsilon_{ik} \phi_k^*) = \delta_{jk} \phi_j \phi_k^* = \phi^\dagger \phi
\end{aligned}
\right. \Rightarrow S^\dagger S = \phi^\dagger \phi \, \mathbb{1} . \tag{A.35}
$$

It follows that: $(\mathrm{Tr}[S^\dagger S])^2 = 4(\phi^\dagger \phi)^2$, $\mathrm{Tr}[S^\dagger S S^\dagger S] = 2(\phi^\dagger \phi)^2$. In conclusion, the most general quartic potential for one single scalar field ϕ is given by:

$$
V = \lambda (\mathrm{Tr}[S^\dagger S])^2 . \tag{A.36}
$$

A.4.2 Multiple scalar fields

In the case of N_S scalar fields ϕ_1, ϕ_2, ... ϕ_{N_S} we define the $2 \times 2N_S$ matrix S as:

$$
S = (\phi_1, \tilde{\phi}_1, \ldots, \phi_{N_S}, \tilde{\phi}_{N_S}) . \tag{A.37}
$$

A gauge transformation is expressed as:

$$
S \to S' = US , \quad \text{with} \quad U \in \mathrm{SU}(2) . \tag{A.38}
$$

S and S^* are related to each other by:

$$
S^* = -\epsilon S E \tag{A.39}
$$

where, in this case:

$$E = \mathrm{diag}(\epsilon, \ldots, \epsilon)\,. \tag{A.40}$$

The kinetic term is expressed as: $\mathcal{L}_{kin} = \frac{1}{2}\mathrm{Tr}\big[(D_\mu S)^\dagger (D^\mu S)\big]$. The constraint A.39 restricts flavour transformation to be: $S \to S' = SM$, with $M \in \mathrm{Sp}(2N_S)$. Given these definitions, the same arguments of equations A.32, A.33, A.34 apply, to show that the most general quartic potential for N_S scalar fields is:

$$V = \lambda_1\big(\mathrm{Tr}\big[S^\dagger S\big]\big)^2 + \lambda_2 \mathrm{Tr}\big[S^\dagger S S^\dagger S\big]\,. \tag{A.41}$$

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