Constraining a fourth generation of quarks: 
non-perturbative Higgs boson mass bounds

J. Bulava, K. Jansen, and A. Nagy

1 CERN, Physics Department, 1211 Geneva 23, Switzerland
2 NIC, DESY, Platanenallee 6, D-15738 Zeuthen, Germany
3 Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, D-12489 Berlin, Germany

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We present a non-perturbative determination of the upper and lower Higgs boson mass bounds with a heavy fourth generation of quarks from numerical lattice computations in a chirally symmetric Higgs-Yukawa model. We find that the upper bound only moderately rises with the quark mass while the lower bound increases significantly, providing additional constraints on the existence of a straightforward fourth quark generation. We examine the stability of the lower bound under the addition of a higher dimensional operator to the scalar field potential using perturbation theory, demonstrating that it is not significantly altered for small values of the coupling of this operator. For a Higgs boson mass of \( \sim 125 \text{GeV} \) we find that the maximum value of the fourth generation quark mass is \( \sim 300 \text{GeV} \), which is already in conflict with bounds from direct searches.

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INTRODUCTION

A heavy fourth generation of quarks is an attractive and simple extension (denoted SM4) of the three-generation Standard Model (SM3) \(^1\), \(^2\). However, heavy fermion effects are expected to significantly contribute to the properties of the Higgs boson, leading to measurable deviations in Higgs production cross sections and branching ratios. The recent discovery of a scalar boson seemingly consistent with the Standard Model expectation therefore casts serious doubt on straightforward fourth generation scenarios \(^3\).

Another property of the Higgs boson which is sensitive to a possible fourth generation is its mass. Invoking arguments from perturbation theory, the Higgs boson mass is bounded from above by the triviality bound, which reflects the Gaussian nature of the UV fixed point, and from below by the vacuum instability bound, which ensures that the theory has a stable vacuum state.

In perturbation theory, the lower bound can be obtained by examining the effective potential and demanding that it remains bounded from below. As the fermion fields contribute negatively to the effective potential, they have a destabilizing effect which leads (by demanding the stability of the theory) to a lower Higgs boson mass bound. However it is expected that the perturbative expansion breaks down for Yukawa couplings near or less than the perturbative unitarity bound \(^4\), which allows maximal fermion masses of roughly \( m_f \approx 500 - 600 \text{GeV} \) \(^5\), \(^6\).

Due to these considerations, study of heavy fourth generation extensions to the Standard Model necessitates non-perturbative methods. To this end, we employ lattice field theory techniques which allow us to compute lower and upper Higgs boson mass bounds as well as resonance parameters of the Higgs boson non-perturbatively. Such a strategy has already been applied in Refs. \(^7\) \(^10\) for the non-perturbative determination of the upper and lower Higgs boson mass bounds and the Higgs boson resonance parameters in the SM3. First results for a fourth quark generation have been presented in Ref. \(^11\). Investigations of a bulk-phase transition at very large values of the Yukawa coupling have been initiated in Ref. \(^12\) while first studies of the system at non-zero temperatures can be found in Ref. \(^13\). For a summary of recent work on this model see Ref. \(^14\).

The lattice calculations are possible due to a lattice discretization of the fermion action which respects an exact chiral symmetry at finite lattice spacing \( a \) \(^15\), thus ensuring that the chiral character of the Higgs-fermion couplings is respected by the lattice regulator in a conceptually clean manner. This advance has triggered a number of lattice investigations of Higgs-Yukawa like models \(^7\), \(^8\), \(^9\), \(^16\), \(^21\).

In this letter we report on a systematic investigation of the lower and upper Higgs boson mass bounds for quark masses ranging from the Standard Model top quark mass of \( m_t = m_t \approx 175 \text{GeV} \) up to masses of \( m_f \approx 700 \text{GeV} \), which is above the perturbative unitarity bound. Our calculations are performed at a fixed lattice cutoff of \( \Lambda = \frac{a}{1.5 \text{TeV}} \) which ensures that the fermion and Higgs boson masses are sufficiently far from the cutoff scale. We also rely heavily on the techniques and simulation strategies of Refs. \(^7\) \(^10\).

Our results indicate that with increasing quark mass there is a substantial upward shift of the lower Higgs boson mass bound leading to severe constraints on a straightforward fourth quark generation in light of the...
recently discovered scalar boson when interpreted as the Standard Model Higgs boson. In order to examine the stability of our results, we analyze the effect of including a higher dimensional operator in the scalar field potential using perturbation theory. For small values of the coupling of this term we confirm that the lower bound is not significantly altered.

THE MODEL

Here we briefly review the definition of our model. For a more complete treatment, see Ref. [9]. We employ a lattice discretization of the Standard Model Higgs-fermion sector which exactly respects a chiral symmetry at finite lattice spacing. As the dynamics of the complex scalar (Higgs) doublet are expected to be dominated by its interactions with the heaviest fermions, we consider a single degenerate quark doublet only. By the same reasoning, the modifications introduced above obey an exact global SU(2)_L × U(1)_Y lattice chiral symmetry. For Ω_L ∈ SU(2) and θ ∈ [0, 2π] the action is invariant under the transformation

\[
\psi \to U_Y \hat{P}_+ \psi + U_Y \Omega_L \hat{P}_- \psi,
\]

\[
\bar{\psi} \to \bar{\psi} \Omega_L^\dagger U_Y^\dagger \hat{P}_- \bar{\psi},
\]

\[
\phi \to U_Y \phi \Omega_L^\dagger, \phi^\dagger \to \Omega_L \phi^\dagger U_Y^\dagger
\]

with \( U_Y \equiv \exp(i\theta Y) \), where \( Y \) labels the representation of the global hypercharge symmetry group U(1)_Y. It should be noted that in the continuum limit the (global) continuum SU(2)_L × U(1)_Y chiral symmetry is recovered.

This formulation enables a numerical study of the limit \( \lambda = \infty \) on the lattice by simply enforcing the constraint \( \Phi^T \Phi = 1 \), \( \forall x \). Also, we can relate the parameters and fields appearing in Eq. (1) to those appearing in the standard scalar complex doublet continuum Lagrangian \( \mathcal{L} = |\partial_\mu \phi|^2 + \frac{1}{2} m_0^2 |\phi|^2 + \lambda |\phi|^4 \) by

\[
\phi_x = \sqrt{2\kappa} \left( \frac{\phi_x^0 + i\phi_x^5}{\phi_x^0 - i\phi_x^5} \right),
\]

\[
\lambda = \frac{\lambda}{4\kappa^2}, \quad m_0^2 = \frac{1 - \frac{\lambda}{8\kappa}}{\kappa}.
\]

COMPUTATIONAL STRATEGY

The cutoff in our model is provided by the inverse lattice spacing (\( \Lambda = 1/a \)) and we set the physical value of \( \Lambda \) using the phenomenological Higgs field vacuum expectation value (vR),

\[
(\sqrt{2G_F})^{-\frac{1}{2}} \approx 246 \text{ GeV} = \frac{v_R}{a} \equiv \frac{v}{\sqrt{Z_G} \cdot a},
\]

where \( Z_G \) denotes the Goldstone boson field renormalization constant and \( v \) the bare scalar field vacuum expectation value. We target a mass range for the degenerate fermion doublet of 175GeV \( \lesssim m_f \lesssim 700 \text{ GeV} \), while fixing the cutoff at \( \Lambda \approx 1.5 \text{ TeV} \). Although the masses of the fermion doublet are degenerate in this work, we plan to assess the effect of a mass splitting in the near future. At \( m_f = m_t = 175 \text{ GeV} \) the splitting \( m_b - m_t \) has been taken into account and found to have a small effect on the lower Higgs boson mass bound which, moreover, can be taken into account by the effective potential evaluated in lattice perturbation theory [7].

We now briefly discuss the simulation algorithm. More details can be found in Ref. [9]. The Monte-Carlo simulations are carried out using a variant [2] of the Hybrid Monte Carlo (HMC) algorithm [23] in which the integration over the Grassmann fields is done analytically at the expense of introducing the determinant of the fermion action in the updating. Therefore, our remaining degrees
of freedom in the Monte Carlo integration are the scalar fields.

Due to the absence of gauge fields, the Overlap operator of Eq. (1) can be constructed exactly in momentum space. However as the Yukawa coupling is local in position space, Fast-Fourier-Transforms (FFT’s) are employed to efficiently apply this term. Finally, Fourier acceleration \(26\) is used to propagate the low momentum modes using coarser time-steps along the HMC evolution, which effectively reduces the autocorrelation between successive scalar field configurations.

It has been demonstrated \(3\) that the Higgs boson mass is a monotonically increasing function of the bare quartic coupling \(\lambda\). Therefore, the lower bound for the Higgs boson mass at fixed cutoff and \(m_f\) is obtained at \(\lambda = 0\), while the upper bound is obtained at \(\lambda = \infty\) \(3\).

Since we work in a finite volume with no external symmetry breaking source, the naively defined vacuum expectation value is zero in an ensemble average. We therefore resort to a special technique, pioneered in Ref. \(27\) and employed in Refs. \(28\) \(30\), of rotating a given scalar field configuration to a preferred direction. It can be shown that in infinite volume this leads to the same vacuum expectation value as obtained in the standard procedure involving the limit of vanishing external source \(30\).

The determination of the Goldstone boson renormalization constant \(Z_G\), the Higgs boson mass \(m_H\), and the fermion mass \(m_f\) have been discussed in detail in Ref. \(8\) and are briefly reviewed here. The renormalization constant \(Z_G\) is computed from the slope of the inverse Goldstone boson propagator at vanishing Euclidean four-momentum transfer, in the standard on-shell scheme. Operationally, this constant is obtained from fits to the propagator at small momenta.

Due to the existence of massless Goldstone modes in the spontaneously broken phase of our theory, the Higgs boson is unstable and can decay to final states containing an even number of Goldstone bosons. We employ two definitions of the Higgs boson mass which both ignore this finite decay width. The Higgs boson propagator mass \(m^P_H\) is derived from fits to the momentum space Higgs propagator defined as

\[
\tilde{G}_H(p) = \langle \tilde{h}_p \tilde{h}_{-p} \rangle, \quad \tilde{h}_p = \frac{1}{\sqrt{L_s \cdot L_t}} \sum_x e^{-ip \cdot \vec{x}} h_x
\]

while the correlator mass \(m^C_H\) is derived from fits to the Higgs temporal correlation function. Although finite decay width corrections to these formulae are quite different, the mass extracted from both of these procedures typically differs by less than 10%, lending credence to our approximation of a stable Higgs boson. Furthermore, a rigorous study of the Higgs boson decay width at non-vanishing external source has been performed at \(m_f = m_t \approx 175\)GeV in Ref. \(10\) which obtained a narrow decay width for all values of the bare quartic coupling, further supporting the validity of the stable Higgs boson approximation. For this work we quote \(m^P_H\) as the central value as it is typically the lowest estimate of \(m_H\).

Finally, we compute the quark mass from the exponential decay of the temporal correlation function \(C_f(t)\) at large Euclidean time separations \(t\), defined as

\[
C_f(t) = \frac{1}{L_s^4 \sum_{x,\vec{y}}} \text{Re} \, \text{Tr} \left( f_{L,0,x} \cdot \tilde{f}_{R,t,\vec{y}} \right),
\]

where the left- and right-handed spinors are defined using the projection operators in Eq. \(2\).

**NUMERICAL RESULTS**

As mentioned above, massless Goldstone excitations are present in the spontaneously broken phase of our model. Since we work at zero external symmetry-breaking source, finite size effects are not exponentially suppressed but rather algebraic in nature and proportional to inverse even powers of the linear extent of the lattice, i.e. \(O(1/L^2)\) at leading order \(28\) \(30\). These finite size effects can be quite substantial and an infinite volume extrapolation of our results for the renormalized vacuum expectation value and all masses is required.

Finite volume data for the Higgs boson propagator mass \(m^P_H\) are shown in Fig. \(1\) as an example of our infinite volume extrapolations. The lattice data are plotted versus \(1/L^2\) and extrapolated to the infinite volume limit by means of a linear fit ansatz according to the aforementioned leading order behaviour. Due to the observed curvature arising from the non-leading finite volume corrections, only those volumes with \(L_s \geq 16\) have been included. One also finds that the infinite volume extrapolation can be reliably performed at ranges of lattice volumes from \(12^3 \times 32\) to \(24^3 \times 32\) if subleading corrections are considered.

The results of the Higgs boson masses for the lower and upper Higgs boson mass bounds as a function of the quark mass at a fixed cutoff of \(\Lambda = 1.5\)TeV are finally presented in Fig. \(2\). All data for the upper bound have been extrapolated to infinite volume, as have the lower Higgs boson mass bounds at \(m_f \approx 160, 192, 420\)GeV Only lower Higgs boson mass bounds at \(m_f \approx 305, 500, 685\)GeV are taken on our presently largest lattice of size \(24^3 \times 32\). However, the finite size corrections of these points will only provide a small change and the behaviour of the lower Higgs boson mass bound as a function of the fermion mass will not be significantly altered.

We find that the upper Higgs boson mass bound is only moderately shifted by about 20% when the fermion mass is increased from \(175\)GeV to \(700\)GeV. On the contrary, the lower Higgs boson mass bound increases drastically with increasing quark mass. Such a significant shift of the lower bound has already been observed in \(7, 8\) for a
quark mass of \( m_f \approx 700\text{GeV} \). We also show in Fig. 2 a lattice perturbative computation of the lower Higgs boson mass bound using the effective potential. The result of this calculation, which is discussed in the next section, is represented by the solid line in Fig. 2. Even up to fermion masses of \( m_f \approx 700\text{GeV} \) the lattice perturbative calculation qualitatively describes the simulation data rather well. This observation allows us to test the stability of the lower bound against the addition of a higher dimensional operator within the framework of the perturbative lattice effective potential. Moreover, direct Monte Carlo simulations with such a term were found to be well-described by perturbation theory within a small range of couplings of this higher dimensional operator.

**EFFECTIVE POTENTIAL**

In addition to non-perturbative numerical data, it is instructive to calculate the lower Higgs boson mass bound perturbatively using the effective potential. To this end we follow Ref. [9] and calculate the effective potential to 1-loop in the large-\( N_f \) expansion.

It should be noted that these calculations are performed with the same lattice regularization used in the simulations maintaining finite spatial and temporal extents. Thus, the loop corrections are calculated numerically, by explicitly performing sums over the lattice momenta. An infinite volume extrapolation of these perturbative results is also performed.

![Figure 1](image1.png)

**FIG. 1:** Infinite volume extrapolation of the Higgs boson mass extracted from fits to the momentum space Higgs propagator \( \langle P H \rangle \). The data are for the Higgs boson mass relevant for the upper bound (\( \lambda = \infty \)) and a range of bare Yukawa couplings corresponding to fermion masses from the physical top quark mass to \( \sim 700\text{GeV} \). The infinite volume extrapolation is performed by fitting the data to a linear function in \( 1/L_s^2 \) taking only data with \( L_s \geq 16 \) into account.

![Figure 2](image2.png)

**FIG. 2:** The lower and upper Higgs boson mass bounds as a function of the fermion mass \( m_f \) for a fixed cutoff of \( \Lambda = 1.5\text{TeV} \). The solid line represents a perturbative lattice effective potential calculation for the lower Higgs boson mass bound.

The vacuum expectation value and lower Higgs boson mass bound are obtained from this effective potential in the usual way, namely

\[
\frac{d}{d\bar{\phi}} V(\bar{\phi})|_{\bar{\phi}=\phi_v} = 0
\]

\[
\frac{d^2}{d\bar{\phi}^2} V(\bar{\phi})|_{\bar{\phi}=\phi_v} = m_H^2,
\]

where \( \bar{\phi} \) denotes the average value of the scalar field. The results of such a determination are shown in Fig. 2. Although quantitatively different, the numerical data agree with the qualitative behaviour of the perturbative result even for rather large fermion masses.

Based on this agreement, we estimate the effect of an additional higher-dimensional operator in the scalar field potential using the perturbative expansion discussed above. To this end we add to Eq. (1) the term \( \lambda_0 \phi^6 \). It has been demonstrated that perturbation theory successfully describes non-perturbative numerical results for the range \( \lambda_0 = [0, 0.01] \). Therefore, at this preliminary stage we examine couplings in this range only. Furthermore, in the presence of such a term we must modify the stability criterion of the effective potential.

Due to the triviality of the theory, the cutoff \( \Lambda \) cannot be completely removed while maintaining non-zero values of the renormalized quartic and Yukawa couplings. However, the existence of a scaling regime suggests that predictions of the model are affected only mildly by small cutoff effects provided that the cutoff is larger than the relevant scales in the theory, namely \( v_R, m_f, m_H \). It has been determined in the pure \( \phi^4 \) theory that a suitable definition of the scaling regime is the situation where \( m/\Lambda < 0.5 \), where \( m = v_R, m_H \). We adopt here this observation also for \( m_f \), keeping \( m_f/\Lambda < 0.5 \).

It is in this scaling regime only that results which are universal up to small cutoff effects can be obtained from our model. Therefore, the vacuum stability criterion
should ensure that a stable vacuum exists throughout the scaling regime. Indeed, the running of the renormalized quartic and Yukawa couplings (and thus vacuum stability considerations) have been demonstrated to be severely regularization dependent outside of the scaling regime defined above [21]. Therefore, we choose as our stability criterion

\[ \frac{d^2}{d\phi^2} V(\phi) > 0, \quad \phi < 0.5. \]  

(7)

In the \( \lambda_6 = 0 \) case, this results in the well-known stability criterion \( \lambda \geq 0 \). We have examined the effect of a finite \( \lambda_6 \) in the range \( \lambda_6 = [0.0, 0.01] \) which results in a less than 1% difference in the lower bound. However for larger values of \( \lambda_6 \sim 0.1 \), deviations as large as 15% have been observed in the lower Higgs boson mass bound. As we are unsure of the applicability of perturbation theory in this region, further non-perturbative numerical simulations must be performed to properly assess the effect of this higher dimensional operator for larger values of \( \lambda_6 \).

OUTLOOK AND CONCLUSIONS

In this letter we have performed a non-perturbative lattice investigation of the lower and upper Higgs boson mass bounds in an extension of the Standard Model with a heavy fourth quark generation. Since the heavy quark masses lead to large values of the Yukawa coupling, such a non-perturbative computation is necessary in order to have reliable results for the Higgs boson mass bounds at large \( m_f \). We include only the dominant interactions, which are expected to be the Higgs-Yukawa interactions of the heavy fermions. In particular, we neglect all gauge fields.

Our chirally invariant lattice regularization of the Higgs-Yukawa sector of the Standard Model (as proposed in Ref. 13) obeys a global \( SU(2)_L \times U(1)_Y \) symmetry at finite lattice spacing, providing a formulation that preserves the chiral nature of the Higgs-fermion couplings.

In this setup, for a fixed cutoff of \( \Lambda = 1 \) TeV, we have studied a range of quark masses \( 175 \) GeV, but will investigate at larger quark masses in the near future.

as previous numerical work, we also used the perturbative effective potential to test the stability of the lower Higgs boson mass bound against addition of a higher dimensional operator for a small range of couplings. We found that the lower Higgs boson mass bound is quite insensitive against such an addition, although more non-perturbative numerical simulations are required to examine the effect of the higher dimension operator for larger couplings. Nonetheless, this preliminary work provides some confidence that the results for the lower bound are robust. Furthermore, although we work with a mass degenerate quark doublet in this work, the dependence of the lower bound on the mass splitting was found to be small at \( m_f = 175 \) GeV, but will investigated at larger quark masses in the near future.

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\[ \text{Electronic address: john.bulava@cern.ch} \]

\[ \text{Electronic address: karl.jansen@desy.de} \]

\[ \text{Electronic address: attila.nagy@physik.hu-berlin.de} \]

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