Numerical simulation of heavy fermions in an SU(2)$_L \otimes$ SU(2)$_R$ symmetric Yukawa model

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Abstract

An exploratory numerical study of the influence of heavy fermion doublets on the mass of the Higgs boson is performed in the decoupling limit of a chiral SU(2)$_L \otimes$ SU(2)$_R$ symmetric Yukawa model with mirror fermions. The behaviour of fermion and boson masses is investigated at infinite bare quartic coupling on 4$^3 \cdot 8$, 6$^3 \cdot 12$ and 8$^3 \cdot 16$ lattices. A first estimate of the upper bound on the renormalized quartic coupling as a function of the renormalized Yukawa-coupling is given.

1 Introduction

Recent LEP measurements [1] fix the number of light neutrinos to three, therefore a simple further repetition of fermion families is excluded. Extensions of the minimal Standard Model by heavy fermions are, however, possible. Examples are: a fourth fermion family with heavy neutrino (for a recent reference see [2]), or a duplication of the three light families by heavy mirror families [3, 4]. Some limitations on the number of heavy fermions follow from studies of 1-loop radiative corrections [5, 6] because of the non-decoupling of heavy fermions. The question of non-decoupling in higher loop orders is, however, open. In fact, one of the goals of lattice studies is to investigate this in the nonperturbative regime of couplings.

The lattice formulation of the electroweak Standard Model is difficult because of the fermion doublers [7]. In fact, at present no completely satisfactory formulation is known [8]: if one insists on explicit chiral gauge invariance, then mirror fermion fields have to be introduced [9], otherwise one has to fix the gauge as in the “Rome-approach” [10]. (In a recently proposed method [11] a fifth extra dimension has to be introduced.)
There is, however, an interesting limit of the Standard Model which can be numerically simulated by present techniques. Namely, if the SU(3) colour \(\otimes\) U(1) hypercharge gauge couplings are neglected, then, as a consequence of the pseudo-reality of SU(2) representations, mirror fermions can be transformed to normal fermions by charge conjugation, and Yukawa models with an even number \(N_f\) of degenerate fermion doublets can be simulated \([8]\). (For instance, \(N_f = 4\) corresponds to a heavy degenerate fermion family.) This can be done at nonzero Yukawa-couplings for both fermion \(G_\psi\) and mirror fermion \(G_\chi\), or by keeping \(G_\chi\) and the fermion-mirror-fermion mixing mass \(\mu_\psi\chi\) at zero, and thereby decoupling the mirror fermion exactly from the physical spectrum \([12]\).

In the present paper we choose this second way, where the exact decoupling in the continuum limit is assured by the Golterman-Petcher fermion shift symmetry \([13]\). This symmetry is exact at \(G_\chi = \mu_\psi\chi = 0\), and implies a set of identities, which makes the parameter tuning easier. Another interpretation of the decoupling limit also deserves attention. Namely, interchanging the rôles of fermion and mirror fermion by considering \(\chi\) to be the fermion and \(\psi\) the mirror fermion, the decoupling scenario turns out to be a rather good approximation of the situation in phenomenological models with mirror fermions \([3]\). This is due to the fact that all known physical fermions have very small Yukawa-couplings. The only fermion states with strong Yukawa-couplings would be the members of the mirror families, if they would exist. In fact, the smallness of the known fermion masses on the electroweak scale could then be explained by the approximate validity of the Golterman-Petcher shift symmetry.

An important set of questions for the numerical simulations is concentrated around the “allowed range of renormalized couplings”, which is cut-off dependent and shrinks to zero for infinite cut-off if the continuum limit is trivial. It is expected on the basis of 1-loop perturbation theory that, as a function of the renormalized Yukawa-coupling, the allowed region for the renormalized quartic coupling is limited by an upper bound obtained at infinite bare quartic coupling \((\lambda = \infty)\), and by a lower bound called “vacuum stability bound” reached at zero bare quartic coupling \((\lambda = 0)\) (for discussions see \([14, 15, 8]\)). In the present work the numerical simulations are restricted to \(\lambda = \infty\), and first results on the behaviour of the upper bound are obtained. The study of the \(\lambda \to 0\) limit is postponed to future work.

### 2 Lattice action, decoupling, physical quantities

Our numerical simulations were performed in the chiral SU(2)_L \(\otimes\) SU(2)_R symmetric Yukawa model with \(N_f = 2\) mirror pairs of fermion doublet fields in the decoupling limit. The conventions in the lattice action and the definition of different renormalized physical quantities closely follow our previous papers on U(1)_L \(\otimes\) U(1)_R \([14, 13]\) and SU(2)_L \(\otimes\) SU(2)_R \([16]\) symmetric models. Therefore we only repeat here the most essential formulae, and include the definitions specific to the present investigation.

The lattice action is a sum of the O(4) \((\cong\text{SU(2)}_L \otimes\text{SU(2)}_R)\) symmetric pure scalar part \(S_\phi\) and fermionic part \(S_\Psi\):

\[
S = S_\phi + S_\Psi.
\]

\(\varphi_x\) is the 2 \(\otimes\) 2 matrix scalar field, and \(\Psi_x \equiv (\psi_x, \chi_x)\) stands for the mirror pair of fermion doublet fields (usually \(\psi\) is the fermion doublet and \(\chi\) the mirror fermion doublet). In the usual normalization conventions for numerical simulations we have

\[
S_\phi = \sum_x \left\{ \frac{1}{2} \text{Tr} (\varphi_x^+ \varphi_x) + \frac{1}{2} \lambda \left[ \frac{1}{2} \text{Tr} (\varphi_x^+ \varphi_x) - 1 \right]^2 - \kappa \sum_{\mu=1}^{4} \text{Tr} (\varphi_{x+\mu}^+ \varphi_x) \right\},
\]
\[
S_\psi = \sum_x \left\{ \mu_\psi \left[ (\overline{\psi}_x \psi_x) + (\overline{\psi}_x \chi_x) \right] - K \sum_{\mu = \pm 1}^{\pm 4} \left[ (\overline{\psi}_x + \bar{\mu} \gamma_\mu \psi_x) + (\overline{\chi}_x + \bar{\mu} \gamma_\mu \chi_x) + r \left( (\overline{\chi}_x + \bar{\mu} \gamma_\mu \chi_x) - (\overline{\psi}_x \psi_x) + (\overline{\psi}_x + \bar{\mu} \gamma_\mu \chi_x) - (\overline{\psi}_x \chi_x) \right) \right] \\
+ G_\psi \left[ (\overline{\psi}_x \bar{\chi}_x \chi_x L_x + (\overline{\psi}_x \bar{\chi}_x \chi_x R_x) \right] + G_\chi \left[ (\overline{\chi}_x \bar{\psi}_x \chi_x L_x) + (\overline{\chi}_x \bar{\psi}_x \chi_x R_x) \right] \right\}.
\]

(2)

Here \( K \) is the fermion hopping parameter, \( r \) the Wilson-parameter, which will be fixed to \( r = 1 \) in the numerical simulations, and the indices \( L, R \) denote, as usual, the chiral components of fermion fields. In this normalization the fermion-mirror-fermion mixing mass is \( \mu_\psi = 1 - 8rK \).

In the limit \( \lambda \to \infty \) the length of the scalar field is frozen to unity, therefore in \( S_\varphi \) only the term proportional to \( \kappa \) is relevant.

The consequence of the Golterman-Petcher identities is that at \( G_\chi = 0 \) all higher vertex functions containing the \( \chi \)-field vanish identically, and the \( \chi \)-\( \chi \)- and \( \chi \)-\( \psi \)-components of the inverse fermion propagator \( \tilde{\Gamma}_\psi(p) \) are equal to the corresponding components of the free inverse propagator [17, 18]). In the broken phase the small momentum \( (p \to 0) \) behaviour of \( \tilde{\Gamma}_\psi \) defines the renormalized \( \psi \)-mass \( \mu_{R\psi} \) and wave function renormalization factor \( Z_\psi \), therefore

\[
\tilde{\Gamma}_\psi(p) \equiv M + i\gamma \cdot p N + O(p^2)
= \begin{pmatrix}
\mu_{R\psi} + i\gamma \cdot \bar{p} + O(p^2) Z_{\psi}^{-1} \mu_0 + \frac{r}{2} \bar{p}^2 \\
\mu_0 + \frac{r}{2} \bar{p}^2 \end{pmatrix}.
\]

(3)

Here \( \mu_0 \equiv \mu_{\psi\chi}/(2K) = (1 - 8rK)/(2K) \) and, as usual, \( \bar{p}_\mu \equiv \sin p_\mu \) and \( \bar{\mu}_\mu \equiv 2 \sin 1/2p_\mu \). The propagator is the inverse of \( \tilde{\Gamma}_\psi \). With the notation

\[
\mu_p \equiv \mu_0 + \frac{r}{2} \bar{p}^2
\]

we have

\[
\tilde{\Delta}_\psi(p) = \tilde{\Gamma}_\psi(p)^{-1} \equiv A - i\gamma \cdot p B + O(p^2) = \left[ (\bar{p}^2 + Z_\psi \mu_p^2)^2 + \mu_{R\psi}^2 \bar{p}^2 \right]^{-1} \cdot \begin{pmatrix}
Z_\psi \mu_p (\bar{p}^2 + Z_\psi \mu_p^2 + i\gamma \cdot \bar{p} \mu_{R\psi}) \\
Z_\psi \mu_p (\bar{p}^2 + Z_\psi \mu_p^2 + i\gamma \cdot \bar{p} \mu_{R\psi}) - Z_\psi \mu_p^2 \mu_{R\psi} - i\gamma \cdot \bar{p} (\bar{p}^2 + \mu_{R\psi}^2 + Z_\psi \mu_p^2) \end{pmatrix} + O(p^2).
\]

(5)

This shows that in the broken phase near \( p = 0 \) the elements of \( \tilde{\Delta}_\psi(p) \) are rapidly changing, unless \( \mu_p \) is very small. Consider, for instance, \( \Delta_{\psi\psi} \):

\[
\tilde{\Delta}_{\psi\psi} = Z_\psi \frac{\mu_{R\psi} \left( 1 + Z_\psi \mu_p^2 \right)^{-1} - i\gamma \cdot \bar{p}}{\bar{p}^2 + Z_\psi \mu_p^2 + \mu_{R\psi}^2 \left( 1 + Z_\psi \mu_p^2 \right)^{-1}} + O(p^2).
\]

(6)

One sees that in the phase with broken symmetry \( (\mu_{R\psi} \neq 0) \) for \( \mu_0 \) and \( p \) both being small there is a qualitative change of the behaviour as a function of \( p \) around \( p^2 \approx \mu_0 \). The limits \( \mu_0 \to 0 \) and \( p \to 0 \) cannot be interchanged. The correct order is to take first \( \mu_0 \to 0 \) and then \( p \to 0 \). Smooth behaviour near \( \mu_0 = 0 \) is reached only if

\[
\mu_0 = O(p^2).
\]

(7)
In this case $\mu_2^2/\bar{p}^2 = O(p^2)$, and the components of the propagator are
\[
\tilde{\Delta}_{\psi\psi}(p) = Z_\psi \frac{\mu R_\psi - i \gamma \cdot \bar{p}}{\mu_2^2 R_\psi + \bar{p}^2} + O(p^2),
\]
\[
\tilde{\Delta}_{\psi\chi}(p) = \tilde{\Delta}_{\chi\psi}(p) = i \gamma \cdot \bar{p} \frac{\mu_2^2 R_\psi}{\bar{p}^2(\mu_2^2 R_\psi + \bar{p}^2)} = O(p),
\]
\[
\tilde{\Delta}_{\chi\chi}(p) = -i \gamma \cdot \bar{p} \frac{\mu_2^2 R_\psi}{\bar{p}^2} + O(p^2).
\] (8)

This limit is best approximated if for a given momentum $p$ we choose
\[
\mu_p = \mu_0 + \frac{r}{2} \bar{p}^2 = 0.
\] (9)

In fact, since our fermionic renormalized quantities are defined at the smallest timelike momentum $p_{\text{min}}$ (and zero spacelike momenta), we took
\[
\mu_{p_{\text{min}}} = 0.
\] (10)

Note that this also implies $\tilde{\Delta}_{\psi\chi}(p_{\text{min}}) = 0$, which ensures that no mixing between $\psi$ and $\chi$ occurs. On a lattice with time extension $T$ the smallest fermion momentum in the timelike direction with our antiperiodic boundary conditions is $p_{\text{min}} = \pi/T$, therefore this condition gives a $T$-dependent hopping parameter $K > K_{\text{cr}} \equiv 1/(8r)$. For $T \to \infty$ one has, of course, $K \to K_{\text{cr}}$.

In summary: since in the broken phase the decoupling situation is reached only for very small $\mu_0$, in terms of the hopping parameter one has to be so close to $K = K_{\text{cr}} \equiv 1/(8r)$ that trying to perform simulations at $K < K_{\text{cr}}$ and to extrapolate to $K = K_{\text{cr}}$ does not pay in the parameter region we studied (see in next section). Therefore in our simulations we always took $\mu_0 \simeq \mu_{p_{\text{min}}} = 0$ ($K \simeq K_{\text{cr}} = 0.125$).

In numerical simulations one can determine the fermion propagator $\tilde{\Delta}_\psi$. For the renormalized quantities one needs the inverse propagator $\tilde{\Gamma}_\psi$. This could, in principle, be obtained for a given momentum by the numerical inversion of the $8 \otimes 8$ matrix in spinor-$\psi$-$\chi$ space, but this would introduce large fluctuations in the results. In [14, 15] we used an analytic inversion up to $O(p^4)$. Here it is better to take
\[
M = (A + \bar{p}^2 B A^{-1} B)^{-1},
\]
\[
N = A^{-1} B M = A^{-1} B(A + \bar{p}^2 B A^{-1} B)^{-1},
\] (11)

which follows from the spinor structure $\tilde{\Delta}_\psi = A - i \gamma \cdot \bar{p} B$, and has at most $O(p^4)$ corrections. In addition, for the exactly known elements of $\tilde{\Gamma}_\psi$ we took the values in [12], and [13] was used only for the $\psi$-$\psi$ component of $\tilde{\Gamma}_\psi$.

The definition of the renormalized physical quantities can be taken over in most cases with trivial modifications from the $U(1)_L \otimes U(1)_R$ model [14, 15]. In the broken phase, where most of our runs were performed, we also use the “constraint correlations” obtained after an SU(2) rotation of the average $\varphi$-field into a fixed (“$\sigma$”) direction. (The three Goldstone boson components of the $\varphi$-field perpendicular to $\sigma$ are denoted by $\pi_a$ ($a = 1, 2, 3$).) In order to avoid infrared singularities, external $\pi$-legs are usually set to the smallest nonzero momentum on our $L^3 \times T$ lattices.

The renormalized Yukawa-couplings can be defined in different ways. One definition is given by the ratio of the mass to the renormalized vacuum expectation value, as for instance
\[ G_{R\psi} = \mu_{R\psi}/v_R. \]

It is interesting to compare this to the renormalized Yukawa couplings obtained through Goldstone-fermion-antifermion vertex functions. These renormalized Yukawa couplings, denoted as \( G_{aR\psi}^{(3)} \) and \( G_{aRx}^{(3)} \), where \( a = 1, 2, 3 \), are defined by

\[
\begin{pmatrix}
  i \gamma_5 \tau_a G_{aR\psi}^{(3)} \\
  0 \\
  -i \gamma_5 \tau_a G_{aRx}^{(3)}
\end{pmatrix}
\delta_{k,-p+q} = \frac{\hat{k}_4^2}{\sqrt{Z_T}} \tilde{\Gamma}_R(p_4) Z^{-1/2}_\psi G_a^{(c)} (Z^{-1/2}_\psi)^T \tilde{\Gamma}_R(q_4),
\]

(12)

where no summation over \( a \) is applied, and \( k_4, p_4, q_4 \) are the 4th components of the momenta of Goldstone boson, fermion and anti-fermion, respectively. We have set the spatial components of all momenta to zero. The appearance of the Kronecker-delta above is due to energy-momentum conservation. The renormalized 2-point fermion vertex function \( \tilde{\Gamma}_R \) at small \( p = (0,0,0,p_4) \) is given as

\[ \tilde{\Gamma}_R(p_4) \simeq i \gamma_4 \bar{p}_4 + M_R, \quad M_R = \begin{pmatrix} G_{R\psi} v_R & \mu_R \\ \mu_R & G_{Rx} v_R \end{pmatrix}, \]

and

\[ G_a^{(c)} = \frac{1}{L^3 T} \sum_{x,y,z} e^{-ik_4 x_4} e^{-ip_4 y_4} e^{iq_4 z_4} \langle \chi_a(x) \Psi(y) \bar{\Psi}(z) \rangle \]

is the connected part of the \( \chi_a^-\Psi^-\bar{\Psi} \) 3-point Green’s function and \( \chi_a(x) \) are the Goldstone fields \( (\Psi(y) \equiv \Psi(y) \) is the fermion field). Using the fact that the renormalized couplings are the same for all three Goldstone bosons, and

\[ \text{Tr}_{\text{Dirac}} (\gamma_5^2) = 4, \quad \text{Tr}_{\text{SU}(2)} (\tau_a \tau_b) = 2\delta_{ab}, \]

we obtain

\[
\begin{pmatrix}
  G_{R\psi}^{(3)} \\
  0 \\
  -G_{Rx}^{(3)}
\end{pmatrix}
\delta_{k,-p+q} = -\frac{i\hat{k}_4^2}{24\sqrt{Z_T}}
\]

\[
\cdot \sum_{a=1}^{3} \text{Tr}_{\text{SU}(2)} \left\{ \tau_a \text{Tr}_{\text{Dirac}} [\gamma_5 \tilde{\Gamma}_R(p_4) Z^{-1/2}_\psi G_a^{(c)} (Z^{-1/2}_\psi)^T \tilde{\Gamma}_R(q_4)] \right\}.
\]

(13)

Because of the existence of massless Goldstone bosons in the broken phase, renormalized quantities cannot be defined at zero momentum. For instance, the connected 3-point \( \chi^-\Psi^-\bar{\Psi} \) Green’s function has an infrared singularity on the external \( \pi \)-leg. Therefore in our simulations on \( L^3 \cdot T \) lattices we choose

\[ k_4 = \frac{2\pi}{T}, \quad p_4 = -\frac{\pi}{T}, \quad q_4 = \frac{\pi}{T}. \]

After carrying out all the matrix multiplications in (13), we get \( G_{R\psi}^{(3)} \) and \( G_{Rx}^{(3)} \). The expressions are too voluminous to be displayed here.

### 3 Numerical simulation

We used the Hybrid Monte Carlo algorithm [18]. This requires the flavour duplication of the fermion spectrum. If the fermion matrix in the action (2) is denoted by \( Q \), then the replica flavours have \( Q^4 \), therefore for them the rôles of \( \psi \) and \( \chi \) are interchanged: \( \chi \) is the “fermion” and \( \psi \) the “mirror fermion”. Since in the model under consideration the fermions are equivalent to mirror fermions, in the decoupling limit \( G_\chi = \mu_\psi = 0 \) the model describes two degenerate fermion doublets (corresponding to the \( \psi \)-fields) and two massless “sterile” doublets (belonging to the \( \chi \)-s), which have no interactions with the physical sector.
The commonly used algorithm for the inversion of the fermion matrix is the conjugate gradient algorithm (CGA). Motivated by the paper of Gupta et al. \[19\] we were also testing matrix inversion by minimal residual algorithm (MRA) with odd-even (o-e) decomposition in our SU(2) symmetric Higgs-Yukawa model with mirror pairs of fermion fields. One difference between our case and that of \[19\] is that we have a nontrivial $Q_{ee}$ and $Q_{oo}$ instead of their matrix $M_1$. But the requirements for a successful implementation of the MRA are satisfied in our case too. Namely we can invert $Q_{ee}$ and $Q_{oo}$ explicitly with an amount of time that is negligible in comparison with the algorithmic inversion of the full matrix $Q$.

To compare the MRA with the CGA we solve the equation $Q + Q_p = v$ for some scalar field configuration $\phi$ at different values of Yukawa-couplings, hopping parameter, lattice size and different convergence parameter. This last quantity is defined by:

$$
\delta = \frac{|Q^+Q_p - v|^2}{|v|^2}. \tag{14}
$$

Using the CGA the solution $p$ is accepted as soon as $\delta$ is smaller than some prescribed $\delta_0$. The solution by MRA is done in two steps, first solving $Q^+\bar{p} = v$ and then $Qp = \bar{p}$, both with a bound for $\delta$ that is a factor of 100 smaller than $\delta_0$.

We were also testing the “polynomial preconditioning” for the MRA, described in \[19\]. Preconditioning of order $n$, denoted by MRA($n$), is characterized by the fact that the matrix, which is to be inverted, contains the fermion hopping parameter $K$ to the power $2n$. The tests were performed at $\lambda = 1.0$ and $\lambda = 10^{-6}$. No important differences were observed for different $\lambda$. As a few test runs showed, at $\lambda = \infty$ the algorithm behaves similarly to $\lambda = 1.0$.

Our results are summarized in tables 1 to 4, where the CPU time necessary for solving $Q^+Q_p = v$ is given in seconds. In these tests we could not find any gain using overrelaxation.

Table 1 shows for $K = 0.1$ that the smaller $\delta_0$ becomes, the better is the MRA compared to CGA. Comparing different preconditionings MRA(1) is the best. This picture changes, if one looks at higher $K$ as can be seen from tables 2 and 3. Near the critical value of $K$ simple preconditioning is no longer the best choice and even with an optimal preconditioning of MRA the CGA performs better.
Table 2: Comparison of matrix inversion algorithms for various $K$. $4^3 \cdot 8$ lattice, $\delta_0 = 10^{-8}$, $G_\psi = 0.3$, $G_\chi = 0.0$, $\kappa = 0.09$, $\lambda = 10^{-6}$.

| $K$   | CGA  | MRA(1) | MRA(2) | MRA(3) |
|-------|------|--------|--------|--------|
| 0.10  | 0.59 | 0.24   | 0.30   | 0.37   |
| 0.11  | 0.87 | 0.35   | 0.41   | 0.59   |
| 0.12  | 1.51 | 0.91   | 1.14   | 1.41   |
| 0.123 | 1.70 | 2.41   | 2.87   | 2.80   |
| 0.124 | 1.74 | 4.37   | 4.45   | 3.90   |

Table 3: Comparison of different preconditionings at $K = 0.125$. $4^3 \cdot 8$ lattice, $\delta_0 = 10^{-8}$, $G_\psi = 0.3$, $G_\chi = 0.0$, $\kappa = 0.09$, $\lambda = 10^{-6}$.

|       | CGA   | MRA(n) |
|-------|-------|--------|
|       | n=1   | 2      | 3      | 4      | 5      | 6      | 7      |
| 1.87  | 11.30 | 8.58   | 6.11   | 3.95   | 2.29   | 12.90  | 15.00  |

Table 4 shows a comparison between MRA and CGA at $K = 0.1$ for different lattice sizes. One observes that the gain of using MRA increases with the lattice size.

Our conclusion is that in the case of small $K$ ($K \leq 0.1$) the MRA has to be preferred. For some choices of parameters, e.g. in the symmetric phase, the gain by using MRA can be so large that it would be advantageous to do calculations at different small values of $K$ (e.g. 0.1, 0.11, 0.12) and then extrapolate to the value under investigation (e.g. 0.125). However for $K$ deep in the broken phase the CGA seems to be still the best choice. For the investigation of the decoupling limit ($K \approx K_{cr} = 0.125$) in the broken phase it was necessary to be very close to $K_{cr}$, and we always used CGA.

The technical advantage of using the decoupling method is that the number of tuned parameters is less, because the fermion hopping parameter is fixed at $K = K_{cr}$. At $\lambda = \infty$ and at a fixed value of the bare Yukawa-coupling $G_\psi$ one has to tune only the scalar hopping parameter $\kappa$. The difficulty is that the presence of massless $\chi$-fermions slows down the convergence of the fermion matrix inversion. We also tried to improve on this by using the free fermion propagator for preconditioning in momentum space. In this way the number of iterations in CGA can be reduced by a factor not larger than two. On the other hand, the computer time required for performing the necessary Fourier transformations is so large that the gain is completely coun-

Table 4: Comparison of matrix inversion algorithms on different lattice sizes $\delta_0 = 10^{-15}$, $G_\psi = 0.1$, $G_\chi = 0.0$, $\kappa = 0.15$, $K = 0.1$, $\lambda = 1.0$.

| $L^3 \cdot T$ | CGA  | MRA(1) | MRA(2) |
|---------------|------|--------|--------|
| $4^3 \cdot 8$ | 0.67 | 0.41   | 0.46   |
| $6^3 \cdot 12$ | 3.84 | 1.97   | 2.24   |
| $8^3 \cdot 16$ | 12.60 | 6.10   | 7.00   |
teracted, except for very small Yukawa-couplings. This is presumably due to the “roughness” of typical scalar field configurations.

Another attempt to improve the matrix inversion was to supply the CGA with an “educated guess” for the start vector in the iterations. This was done by means of a hopping parameter expansion of $Q^{-1}$ up to some order $n$:

$$Q^{-1} \approx Q_n^{-1} = D^{-1} \left(1 - \sum_{k=1}^{n} (MD^{-1})^k\right),$$

where $D$ and $M$ are the diagonal and off-diagonal parts of $Q$ with respect to site indices, and $n$ was optimized for given parameters $K$ and $G_{\psi}$. For $K = 0.1$ and $G_{\psi} < 2.4$ the speed of the algorithm can be increased up to a factor of three in this way. On the other hand, for $K$ above its critical value this improvement is not applicable.

4 Results

The first step in the numerical simulations was to check the phase structure at $\lambda = \infty$ and $K = K_{cr}$. On the basis of experience with several other lattice Yukawa models [17, 21], and our own previous work [21], this is expected to possess several phase transitions between the “ferromagnetic” (FM), “antiferromagnetic” (AFM), “paramagnetic” (PM) and “ferrimagnetic” (FI) phases. The resulting picture in the $(G_{\psi}, \kappa)$-plane is shown in fig. 1. Due to CPU-time limitations we did not try to disentangle the details of the structure near the meeting point of the four phases, neither did we follow the shape of the FI-phase for very strong bare Yukawa-coupling beyond $G_{\psi} = 1.5$.

The physical phase is FM with spontaneously broken chiral symmetry. Therefore we fixed $G_{\psi} = 0.3, 0.6, 1.0$ and performed a series of runs in the $\kappa$-ranges shown in fig. 1 by the dashed lines. Most of the time $4^3 \cdot 8$ and $6^3 \cdot 12$ lattices were taken. In a few particularly important points, for instance at $(\kappa = 0.27, G_{\psi} = 0.3)$ and $(\kappa = 0.15, G_{\psi} = 0.6)$, in addition to $4^3 \cdot 8$ and $6^3 \cdot 12$ also an $8^3 \cdot 16$ run was performed. The typical run consisted of about 1000-2000 equilibrating and 4000-10000 measured HMC trajectories. The length of trajectories was randomly changed by the number of classical dynamics steps between 3 and 10. The step length was chosen such that the average acceptance rate per trajectory stayed near 0.75.

On our lattices the expectation value of the average of the scalar field in the $\sigma$-direction $v \equiv \langle \sigma_x \rangle = \langle \phi_{Lx} \rangle$ (in short “magnetization”) has a smooth behaviour across the physically important PM-FM phase transition (part of our data is shown in fig. 2). Furthermore, the magnetization always decreased with increasing lattice size, in the same way as in case of the pure O(4)-symmetric $\phi^4$ model. This agrees with the expected second order phase transition, which is well suited for the definition of a continuum limit.

In all data points the mass of the mirror fermion, $\mu_{R\chi}$, and the renormalized mixing mass, $\mu_R$, were consistent with zero within errors, in agreement with the consequences of the Golterman-Petcher relations.

The behaviour of the fermion mass $\mu_{R\psi}$ and Higgs-boson mass in lattice units is shown in figs. 3 and 4, respectively. The fermion mass ($\mu_{R\psi}$) is decreasing monotonically to zero, as one approaches the phase transition from the FM-side (decreasing $\kappa$). This agrees with the expectation, since in the PM phase, due to $K \simeq K_{cr}$, the fermion mass is nearly zero (at $K = K_{cr}$ on an infinite lattice it would be exactly zero). At the same time the fermion mass is increasing with $G_{\psi}$, in such a way that at $G_{\psi} = 1.0$ within our limited computer time we were
unable to find points with really small masses. This could presumably be cured by investigating more points on larger lattices. In fact, the fermion mass shows in this point strong finite size effects, implying smaller masses on larger lattices.

The masses of the doubler fermions for both \( \psi \) and \( \chi \) at nonzero corners of the Brillouin-zone were also determined and turned out to be always above 1.5, with a slight decreasing tendency for increasing \( G_\psi \).

The values of the Higgs-boson mass \( (m_{R\sigma} \equiv m_L) \) were determined by fitting the constraint correlation in the \( \sigma \)-channel by a form \( \cosh() + \text{const.} \) in the range \( 1 \leq t \leq T/2 \). The dependence of \( m_{R\sigma} \) on \( \kappa \) in fig. 4 shows a gradual decrease and then a sharp increase for decreasing \( \kappa \). On larger lattices the values are smaller, but there is a substantial increase with increasing \( G_\psi \) if the lattice size is kept fixed. This is depicted in fig. 5, where the averages of a few points with lowest Higgs-boson mass are shown. This figure also displays the strong finite size effects present on these lattices: in the limit of infinitely large volumes the minimum of \( m_{R\sigma} \) is expected to be zero at the second order phase transition between the FM-PM phases. A plausible interpretation of fig. 5 is that the finite size effects become stronger for larger \( G_\psi \), because the renormalized couplings become stronger. In any case, the large values at the minima represent a difficulty for the numerical simulations in the critical region, because large lattices are needed. Our experience shows (see also table 3), that reasonably small masses \( m_{R\sigma} \simeq 0.5 - 0.7 \) can be achieved at \( G_\psi = 0.3 \) on \( 6^3 \cdot 12 \), at \( G_\psi = 0.6 \) on \( 8^3 \cdot 16 \) lattices. Presumably at \( G_\psi = 1.0 \) lattices with spatial extension of at least \( 16^3 \) are necessary. In general, for a physical interpretation of the results in the broken phase on a lattice of given size one should stay with \( \kappa \) above the value where \( m_{R\sigma} \) takes its minimum. This expectation is strengthened by the comparison of \( 6^3 \cdot 12 \) and \( 8^3 \cdot 16 \) results at \( (\kappa = 0.27, G_\psi = 0.3) \), which are both in the broken phase, and within statistical errors show no finite size effects of the renormalized couplings (see below).

The behaviour of the \( \sigma \)- (Higgs-boson) and \( \pi \)- (Goldstone-boson) inverse propagators as a function of momentum is shown at \( G_\psi = 0.6, \kappa = 0.15 \) in fig. 6. The method of measurement is the same as in Ref. [22]. The Goldstone- \( (\pi-) \) and \( \sigma \)-propagators in momentum space are defined by

\[
\tilde{G}_\pi(p) = \left\langle \frac{1}{3L^3} \sum_{x,y} \sum_{a=1}^{3} \pi_{ax} \pi_{ay} \exp\{ip \cdot (x - y)\} \right\rangle, \tag{15}
\]

\[
\tilde{G}_\sigma(p) = \left\langle \frac{1}{L^3} \sum_{x,y} \sigma_x \sigma_y \exp\{ip \cdot (x - y)\} \right\rangle. \tag{16}
\]

In order to limit computer time and storage we actually measure \( \tilde{G}(p) \) for only one of multiple 4-momenta \( p \) giving degenerate \( \tilde{p}^2 \) according to the assumption that, at least for small momenta, \( \tilde{G}(p) \) is just a function of \( \tilde{p}^2 \). The values are blocked during the MC runs with a block length of typically 100 configurations. The error bars are estimated with the jackknife method. As one can see, in this point the inverse \( \pi \)-propagator extrapolates reasonably well to zero for zero momentum. The extrapolation of the inverse \( \sigma \)-propagator to zero gives a Higgs-boson mass \( m_{R\sigma} = 0.98 \pm 0.05 \), in good agreement with the value obtained from a fit of the time-dependence of timeslices. The curvature of the inverse propagators at this \( (\kappa, G_\psi) \) value is not strong. This allows a reasonably accurate determination of the renormalized quantities by the formulae in [13], assuming a linear dependence between zero and the lowest nonzero momentum. For larger values of the momentum the propagators are quite smooth, therefore the effect of heavy \( \psi \)-fermion doublers is not strong. Closer to the phase transition the curvature of the inverse propagators near zero momentum becomes stronger, and the \( \pi \)-propagator starts to show an increasingly nonzero mass. We interpret the latter as a finite size effect.
Taking the Goldstone-boson field renormalization factor \( Z_\pi \equiv Z_T \) from the \( \pi \)-propagator, one can determine the renormalized scalar vacuum expectation value \( v_R = \langle \sigma_x \rangle / \sqrt{Z_\pi} \), which in turn gives the renormalized quartic- \((g_R)\) and Yukawa-couplings \((G_{R\psi})\) by

\[
g_R \equiv \frac{3m_{R\sigma}^2}{v_R^2}, \quad G_{R\psi} \equiv \frac{\mu_{R\psi}}{v_R}.
\]

These are shown in figs. 7 and 8. Although the errors are quite large, one can observe a strong increase of \( g_R \) for decreasing \( \kappa \). In the \( \kappa \) region above the minimum of \( m_{R\sigma} \) there is much less variation. The values on these “plateaus” show a moderate increase for increasing \( G_{R\psi} \). The renormalized Yukawa-coupling \( G_{R\psi} \) is rather flat as a function of \( \kappa \), but increases definitely with \( G_{\psi} \).

Considering only the points above the minimum of \( m_{R\sigma} \) on the given lattice size as being in the broken phase, one can make a tentative first estimate of the upper bound on the renormalized quartic coupling (or Higgs-boson mass), as a function of the renormalized Yukawacoupling (or fermion mass). Such an estimate is shown by fig. 9 together with the perturbative estimates based on the 1-loop \( \beta \)-functions. The agreement with the perturbative results at \( G_{\psi} = 0.3 \) and 0.6 is good, although the renormalized couplings are quite strong, i.e. close to the tree unitarity bound. The \( 8^3 \cdot 16 \) points have, unfortunately, larger statistical errors. At strong coupling the good agreement could partly be due to a fixed point in the ratio \( g_R/G_{R\psi}^2 \), which implies that this ratio is insensitive to the cut-off.

A few measured physical quantities in selected typical points are collected in table 5. Comparing the results at \( G_{\psi} = 0.6, \kappa = 0.15 \) on \( 4^3 \cdot 8, 6^3 \cdot 12 \) and \( 8^3 \cdot 16 \) lattices with label b, c and d, respectively, one can see the evolution of the finite size effects. Between c and d there is much less change than between b and c, but point d on the \( 8^3 \cdot 16 \) lattice still does somewhat differ from the infinite volume limit. This may explain why the corresponding point in fig. 9 is higher than the \( 6^3 \cdot 12 \) points at larger \( \kappa \). The situation is better if one compares points C and D, where the deviation of the renormalized couplings is within statistical errors.

A qualitative relation of the masses at the strongest Yukawa-coupling \( (G_{\psi} = 1.0) \) is that the mass of the Higgs-boson \( m_{R\sigma} \) is roughly twice as large as the fermion mass \( \mu_{R\psi} \). Because of finite size effects and limited statistics it cannot be decided at present whether the \( \sigma \)-particle is a two-fermion bound state or a resonance near threshold. In the latter case, due to the fast decay into a fermion pair, the physical Higgs-boson could become a very broad resonance.

An interesting question is the behaviour of the renormalized Yukawa-coupling \( G_{R\psi}^{(3)} \) defined by the 3-point vertex function in (13). \( G_{R\psi}^{(3)} \) is smaller than \( G_{R\psi} \) in all points. The measured values on \( 6^3 \cdot 12 \) lattice are, for instance, \( G_{R\psi}^{(3)} = 1.0 \pm 0.6 \) at point c and \( G_{R\psi}^{(3)} = 1.8 \pm 0.5 \) at point a. Therefore the ratio

\[
S_3 \equiv \frac{G_{R\psi}^{(3)}}{G_{R\psi}}
\]

is smaller than 1. On the \( 8^3 \cdot 16 \) lattice, within our statistics \( G_{R\psi}^{(3)} \) turned out to be difficult to measure. An exception is point D where we obtained \( G_{R\psi}^{(3)} = 0.74 \pm 0.05 \). This is also smaller by about a factor of 2 than the corresponding value of \( G_{R\psi} \). The deviation could partly be due to the nonzero momentum value where \( G_{R\psi}^{(3)} \) was extracted.

The measured values of \( G_{R\chi} \) were always consistent with zero within small errors, in agreement with the consequences of the Golterman-Petcher relations.
Table 5: The main renormalized quantities and the bare magnetization $\langle \sigma \rangle \equiv \langle |\varphi| \rangle$ for several bare couplings $G_\psi$, and $\kappa$-values near the minimum scalar mass attainable for the given lattice size. Points labelled by capital letters are at $G_\psi = 0.3$, whereas lower case and greek letters denote data obtained for $G_\psi = 0.6$ and $G_\psi = 1.0$, respectively.

| $L^3 \cdot T$ | $\kappa$ | $\langle \sigma \rangle$ | $v_R$ | $m_{R\sigma}$ | $\mu_{R\psi}$ | $g_R$ | $G_{R\psi}$ |
|---------------|----------|-----------------|-------|--------------|-------------|------|-------------|
| A 4$^3 \cdot 8$ | 0.24 | 0.2807(15) | 0.307(4) | 1.23(1) | 0.34(2) | 48(3) | 1.09(7) |
| B 6$^3 \cdot 12$ | 0.24 | 0.146(6) | 0.18(1) | 0.73(5) | 0.21(4) | 53(16) | 1.2(4) |
| C 6$^3 \cdot 12$ | 0.27 | 0.303(3) | 0.309(13) | 0.80(5) | 0.39(2) | 20(4) | 1.25(5) |
| D 8$^3 \cdot 16$ | 0.27 | 0.270(2) | 0.25(1) | 0.77(3) | 0.34(2) | 31(4) | 1.35(6) |
| E 6$^3 \cdot 12$ | 0.30 | 0.4391(14) | 0.400(13) | 1.17(7) | 0.55(2) | 26(7) | 1.36(6) |
| a 8$^3 \cdot 16$ | 0.12 | 0.118(5) | 0.136(15) | 0.63(8) | 0.61(2) | 80(50) | 4.5(3) |
| b 4$^3 \cdot 8$ | 0.15 | 0.3358(16) | 0.361(8) | 1.60(6) | 1.9(3) | 59(7) | 4.9(5) |
| c 6$^3 \cdot 12$ | 0.15 | 0.248(2) | 0.25(1) | 1.14(5) | 0.67(6) | 63(10) | 2.7(3) |
| d 8$^3 \cdot 16$ | 0.15 | 0.218(3) | 0.217(17) | 0.86(6) | 0.54(4) | 52(9) | 2.5(3) |
| e 6$^3 \cdot 12$ | 0.18 | 0.3524(18) | 0.36(2) | 1.23(8) | 0.86(8) | 36(6) | 2.4(3) |
| f 6$^3 \cdot 12$ | 0.21 | 0.4390(17) | 0.41(2) | 1.34(8) | 1.11(3) | 32(5) | 2.71(13) |
| $\alpha$ 6$^3 \cdot 12$ | $-0.12$ | 0.189(2) | 0.243(14) | 1.79(15) | 0.95(9) | 180(40) | 3.9(4) |

5 Conclusions

The important trends seen in our numerical data on 4$^3 \cdot 8$, 6$^3 \cdot 12$ and 8$^3 \cdot 16$ lattices are the following:

- The phase structure at $(\lambda = \infty, K = K_{cr})$ is qualitatively the same as in other lattice Yukawa-models with FM, PM, AFM and FI phases (fig. 1).

- The FM-PM phase transition at $\lambda = \infty$ is smooth, probably of second order (fig. 2).

- On most of our lattices there are strong finite size effects. In particular, large lattices are needed in order to bring the minimum of the Higgs-boson mass on a given lattice size down to interesting values below 1. As our simulations show, at moderate values of the bare Yukawa-coupling 8$^3 \cdot 16$ might be enough, but for large values near $G_\psi \geq 1.0$ one will need at least presumably something like 16$^3 \cdot 32$.

- Considering only the $\kappa$-values above the minimum of the Higgs-boson mass on a given lattice size, where in one point we also have evidence that finite size effects are not very strong, we obtained a first tentative estimate of the upper bound on the renormalized quartic coupling as a function of the renormalized Yukawa-coupling (fig. 9). Up to renormalized Yukawa-couplings at the tree unitarity limit, which is reached near $G_\psi = 0.6$, this agrees well with 1-loop perturbation theory, but further investigations are necessary in order to check finite size effects and extend the results towards larger $G_\psi$.

- At the strongest Yukawa-coupling $G_\psi = 1.0$ the mass of the physical Higgs-boson is roughly equal to twice the heavy fermion mass. This could imply that the Higgs-boson is a very broad resonance, which decays very fast into a heavy fermion pair.
For a given lattice size the renormalized Yukawa-coupling $G_{R\psi}$ defined by the fermion mass increases more or less linearly with $G_\psi$ up to $G_\psi = 1.0$, where it becomes almost twice the tree unitarity bound $\simeq 2.5$. $G_R^{(3)}$ defined by the 3-point vertex function is smaller than $G_{R\psi}$ on the $6^3 \cdot 12$ and $8^3 \cdot 16$ lattices. As discussed above, the finite size effects are particularly strong for $G_\psi > 0.6$, therefore large lattices are needed for confirmation of the values of $G_{R\psi}$.

The question of the possible influence of heavy fermions in the Standard Model is important and very interesting. By numerical simulations at $\lambda = \infty$ one can obtain information on the upper limit on the Higgs-boson mass. The extension to smaller values of the bare quartic coupling, in particular to $\lambda \simeq 0$ gives a lower bound related to vacuum stability.

Note added: In writing this paper we received a recent preprint of Bock, Smit and Vink, where the same continuum “target” theory as ours has been numerically investigated in a staggered fermion formulation [23].

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**Figure captions**

**Fig. 1.** Phase structure of the $\text{SU}(2)_L \otimes \text{SU}(2)_R$ symmetric Yukawa model at $\lambda = \infty$ in the $(G_\psi, \kappa)$-plane. The remaining bare parameters are fixed by the conditions $\mu_p = 0$, $G_\chi = 0$. Open circles denote points in the PM phase, crosses represent points in the FM phase. The points in the AFM and FI phases are denoted by full circles and open squares, respectively. The dashed lines labelled R,S,T each show the range of $\kappa$ used for a systematic scan of renormalized parameters at fixed $G_\psi$. The crosses along those lines denote the $\kappa$ values where the minimum scalar mass in the broken phase is encountered. Solid lines connect the critical values for $\kappa$ estimated from the behaviour of $\langle \sigma \rangle^2$ on $4^3 \cdot 8$. Dashed lines around the FI phase show the expected continuation of the critical lines.

**Fig. 2.** The square of the magnetization as a function of $\kappa$. Here and in the following figures, points at $G_\psi = 0.3$ are represented by triangles, points at $G_\psi = 0.6$ by squares and points at $G_\psi = 1.0$ by circles. Open symbols denote the $4^3 \cdot 8$ lattice, whereas filled-in symbols stand for points obtained on $6^3 \cdot 12$.

**Fig. 3.** The fermion mass $\mu_{R\psi}$ plotted versus $\kappa$ for $G_\psi = 0.3$ (triangles) and $G_\psi = 0.6$ (squares) on lattices of size $4^3 \cdot 8$ (open symbols) and $6^3 \cdot 12$ (filled-in symbols). Errorbars are omitted when the variation is of the size of the symbols. It is seen that larger bare couplings $G_\psi$ in general yield larger fermion masses.

**Fig. 4.** The scalar mass $m_{R\sigma}$ plotted versus $\kappa$. The explanation of symbols corresponds to fig. 3. When approaching the phase transition the scalar masses increase again after going through a minimum.

**Fig. 5.** The minimum of the scalar masses for different $G_\psi$ on $4^3 \cdot 8$ (open symbols) $6^3 \cdot 12$ (filled-in symbols) and $8^3 \cdot 16$ (square plus vertex). The $G_\psi$-values of the two points at $G_\psi = 1.0$ are slightly shifted in the plot to give a better separation.

**Fig. 6a.** The inverse propagator for the massive scalar field (open squares) and the massless components (crosses) plotted versus the square of the lattice momentum $\hat{p}$. The observed curvature is caused by the interaction with fermions.

**Fig. 6b.** The inverse $\pi$-propagator from fig. 6a for the first few lattice momenta. The inverse of the renormalization constant $Z_T$ is in principle determined by the slope of the curve through the origin, and is approximated by the slope of the straight line through the origin and the point with smallest nonzero momentum, as shown by the dotted line.

**Fig. 6c.** The inverse $\sigma$-propagator from fig. 6a for the first few lattice momenta. Extrapolating the curve to zero momentum gives an estimate for $m_{R\sigma}^2$.

**Fig. 7.** The renormalized Yukawa-coupling $G_{R\psi}$ versus $\kappa$ for different bare $G_\psi$. The explanation of symbols is the same as in fig. 2.
**Fig. 8.** The renormalized quartic coupling $g_R$ as a function of $\kappa$ for three different bare values of $G_\psi$.

**Fig. 9.** The renormalized quartic coupling $g_R$ plotted versus $G^2_{R\psi}$. Full data points are from runs on $6^3 \cdot 12$ and represent the mean values obtained from the data points C,E and e,f in table 3 respectively. In addition, two runs on $8^3 \cdot 16$ are shown, namely point D (open triangle plus vertex) and point d (open square plus vertex). The solid and dotted curves show the results for the upper bound on $g_R$ computed from the integration of the 1-loop $\beta$-functions for a scale ratio $\Lambda/m_{R\sigma} = 3, 4$, respectively. The first value for $\Lambda/m_{R\sigma}$ corresponds to $m_{R\sigma} \simeq 1$ in lattice units, whereas the latter is equivalent to $m_{R\sigma} \simeq 0.75$. (The cut-off $\Lambda$ is defined to be $\pi$ in lattice units.)