1 Computational algorithm

1.1 Rational Hybrid Monte Carlo

The overlap fermion operator of the Top-Higgs Yukawa model is given by $\mathcal{M} = D + g\phi\,(1 - D)$. $g\phi$ and D do not commute, so $\mathcal{M}$ is not γ_5 hermitian; however, the underlying Hamiltonian of the continuum theory has charge conjugation symmetry and so the eigenvalues of $\mathcal{M}$ are either real or complex conjugate-paired. Positivity of the determinant is not guaranteed, .../???. To represent a single Top flavor in the model, we replace $\det \mathcal{M}$ with $\det(\mathcal{M}\mathcal{M}^\dagger)^{1/2}$ in the pseudofermion action.

The Hybrid Monte Carlo (HMC) algorithm is the *de facto* algorithm for fermion theories without rooting. Rational Hybrid Monte Carlo (RHMC) [1] augments HMC with optimal rational approximation to accomplish the rooting in our model. The fermion determinant is calculated in terms of pseudofermions as

$$\det \mathcal{M} = \det(\mathcal{M}\mathcal{M}^\dagger)^{1/2} = \int D\chi^\dagger\ D\chi\ e^{-\chi^\dagger(\mathcal{M}\mathcal{M}^\dagger)^{-1/2}\chi} = \int D\chi^\dagger\ D\chi e^{-S_T} \tag{1.1}$$

The momentum conjugate to the Higgs field is introduced in order to define a Hamiltonian, $H = \frac{1}{2}Tr\pi^2 + S_\phi + S_T$. The Higgs field is evolved by numerically integrating the equations of motion with finite timestep, $\Delta\tau$,

$$\frac{\Delta\phi}{\Delta\tau} = \pi \quad , \qquad \frac{\Delta\pi}{\Delta\tau} = -\frac{\partial S}{\partial\phi} \tag{1.2}$$

This is termed molecular dynamics (MD). The MD introduces an $O(\Delta\tau^k)$ error into the probability distribution, where k is the order of the integration scheme used. This error is eliminated by applying a Metropolis acceptance test which defines the end of a trajectory. The Metropolis scheme requires detailed balance, which is provided if the MD integration scheme is reversible (or symmetric) and area-preserving (i.e., symplectic). Ergodicity comes from refreshing the conjugate momentum and pseudofermion fields at the beginning of each trajectory. In our implementation, we generate these pseudorandomly each time with distributions

$$P(\pi) \propto e^{-\pi^*\pi/2} \tag{1.3}$$

and

$$P(\chi) \propto e^{-S_T}. \tag{1.4}$$

We accomplish the latter distribution in the usual manner. We generate a Guassian-distributed vector ξ, i.e. $P(\xi) \propto e^{-\xi^*\xi}$, and then compute χ as $(\mathcal{M}\mathcal{M}^\dagger)^{-1/4}\xi$. The Metropolis component of HMC removes the stepsize dependence of the procedure, yielding an exact algorithm. The stepsize is chosen to reduce autocorrelations, which lessen non-trivially as trajectory length and acceptance rate are increased.

The roots in S_T and in the pseudofermion generation are treated with optimal rational approximations. Using the Remez algorithm, we compute the residues α and poles β of the m-degree partial fraction expansions,

$$(\mathcal{M}\mathcal{M}^\dagger)^\rho \approx \alpha_0^{(\rho)} + \sum_{k=1}^{m} \frac{\alpha_k^{(\rho)}}{\mathcal{M}\mathcal{M}^\dagger + \beta_k^{(\rho)}}. \tag{1.5}$$

Serendipitously, for $|\rho| < 1$ the residues and poles are always positive, so the approximation is stable and also ammenable to the multi-shift conjugate gradient method [2]. Using this method, the entire approximation can be evaluated for nearly the same processing cost as a single matrix inversion (however, the memory requirement can be considerable). Furthermore, evaluating the pseudofermion force as a derivative of the approximation allows for an efficient summation of HMC-like terms,

$$S_T' = -\sum_{k=1}^{m} \alpha_k^{(-1/2)} \chi^\dagger(\mathcal{M}\mathcal{M}^\dagger + \beta_k^{(-1/2)})^{-1}(\mathcal{M}\mathcal{M}^\dagger)'(\mathcal{M}\mathcal{M}^\dagger + \beta_k^{(-1/2)})^{-1}\chi \tag{1.6}$$

Now, unlike the case of PHMC, we must enforce the degeneracy condition with a rational kernel to allow the heatbath to be evaluated. The great advantage, though, is that there is no requirement to reweight the acceptance test because we can include a rational approximation to arbitrary precision. Hence we may proceed exactly as in conventional HMC.

1.2 Fourier space overlap operator

The "outer inversion" of the fermion operator $\xi = (\mathcal{M}\mathcal{M}^\dagger)^{-1}\chi$ takes n_{outer} CG steps as usual, but the usual "inner inversion," to evaluate the Zolotarev optimal approximation to the sign function in the overlap operator, is not necessary. With no gauge field, the massless overlap operator is diagonal in Fourier space, allowing a different approach. As described in [3], it is substantially more efficient to FFT a pseudofermion to momentum space, apply the diagonal overlap operator, and inverse FFT back to position space than to invert. We use FFTW3 [4] which implements SSE macros and multithreading. This procedure does not work in the presence of gauge link variables.

1.3 Fourier acceleration

The absence of gauge fields and computing the overlap in Fourier space lead one to consider applying Fourier acceleration, described superbly by Catterall [5]. In our equivalent picture, we introduce a so-called conjugate mass field $\tilde{m}(p)$ in Fourier space with the intention of compensating for the momentum dependence of the Higgs and pseudofermion forces in the MD, which in turn reduces autocorrelations. The conjugate mass enters the RHMC algorithm in several places. Foremost, the equations of motion become

$$\frac{\Delta\tilde{\phi}}{\Delta\tau} = \frac{\tilde{\pi}}{\tilde{m}} \quad , \qquad \frac{\Delta\tilde{\pi}}{\Delta\tau} = -\mathrm{fft}\left(\frac{\partial S}{\partial\phi}\right). \tag{1.7}$$

Of course, this demands the MD Hamiltonian take the form

$$H = \frac{1}{2}\sum_{p\in\mathcal{B}}\frac{\tilde{\pi}^2}{\tilde{m}} + S_\phi + S_T, \tag{1.8}$$

and furthermore the conjugate momentum must be generated according to

$$P(\tilde{\pi}) \propto e^{-\tilde{\pi}^*\tilde{\pi}/2\tilde{m}}. \tag{1.9}$$

All else is unchanged.

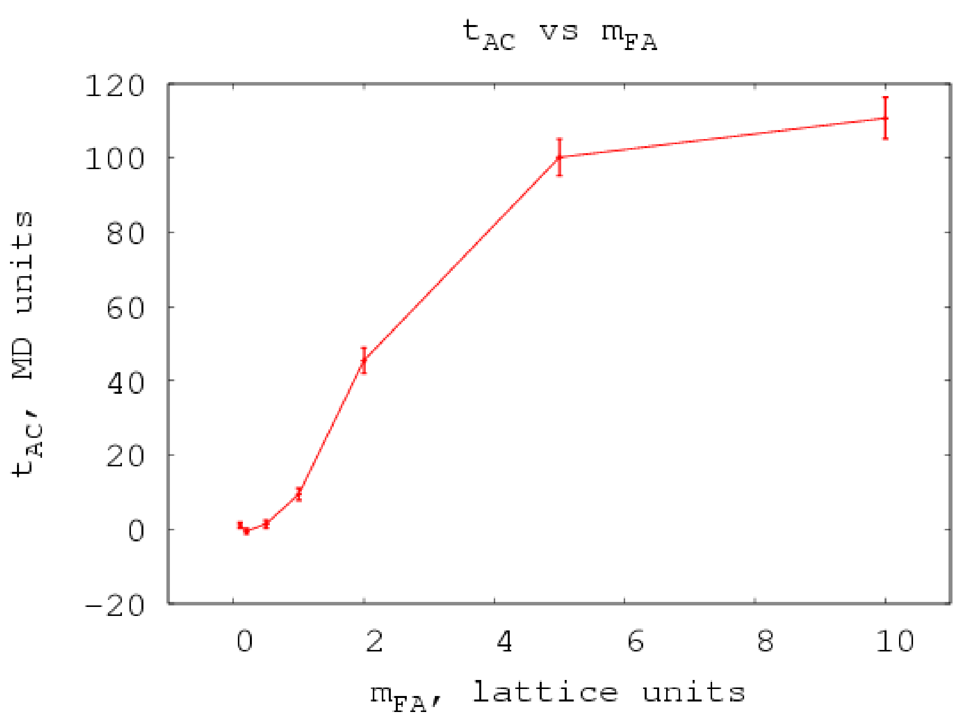

Figure 1: Autocorrelation time dependence on Fourier acceleration parameter m_{FA}.

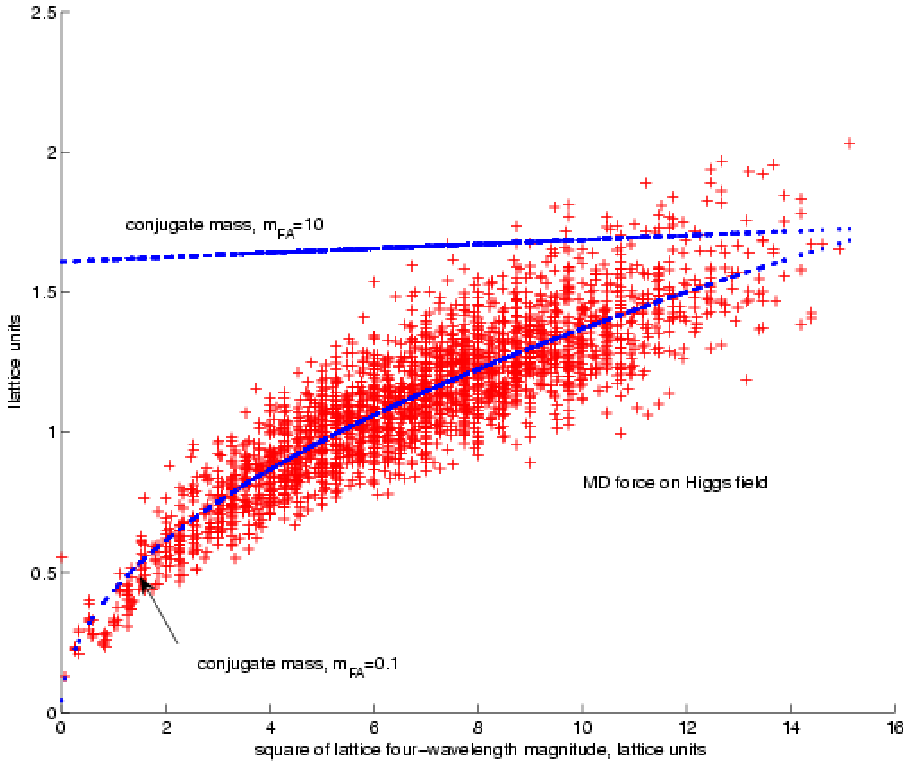

Figure 2: Higgs force profile in momentum space (red) with conjugate mass for $m_{\rm FA} = 10.0$, 2.0, and 0.2 (blue).

As Catterall suggests, the square root of the Higgs propagator serves as a fine first approximation to the momentum dependence of the force on the Higgs field, leading to the form,

$$\tilde{m}(p) = \frac{m_{\rm FA}^2 + \hat{p}^2}{m_{\rm FA}^2 + 16.d0}. \tag{1.10}$$

where $\hat{p}_\mu = 2\sin(p_\mu/2)$ and $m_{\rm FA}$ is a parameter which is tuned to optimize the method. In a free theory, $m_{\rm FA}$ should be set to the bare lattice mass; for an interacting theory, the vicinity of the mass gap is suitable. In an exploratory study on a $12^3 \times 24$ lattice, we found that this prescription works very well. As $m_{\rm FA}$ is decreased from 10.0 (virtually no Fourier acceleration) to 0.2, the autocorrelation is reduced from 111 MD time units to within error of none at all, as shown in Figure 1. In this study, $m_{\rm FA}$ below 0.10 gave unwieldy molecular dynamics and poor acceptance rates. Figure 2 shows that the form Equation 1.10 with $m_{\rm FA} = 0.20$ does indeed fit the force profile well.

critical exponent???

References

[1] A. D. Kennedy, arXiv:hep-lat/0607038. S. Duane, A. D. Kennedy, B. J. Pendleton and D. Roweth, Phys. Lett. B **195**, 216 (1987).

[2] B. Jegerlehner, arXiv:hep-lat/9612014.

[3] P. Gerhold and K. Jansen, arXiv:0705.2539 [hep-lat].

[4] M. Frigo and S. G. Johnson, Proc. IEEE 93 (2) (2005) 216-231.

[5] S. Catterall and S. Karamov, Phys. Lett. B **528**, 301 (2002) [arXiv:hep-lat/0112025].