Automated Perturbation Theory for staggered and minimally doubled fermions

G.M. von Hippel







Mainz Institute of Theoretical Physics Johannes Gutenberg-Universität Mainz

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- Feynman rules become very complex
 - $U_{\mu}(x) = e^{igaA_{\mu}(x+\frac{1}{2}\hat{\mu})} \Rightarrow$ vertices of arbitrary adicity
 - $\bullet~$ Discrete Fourier-transform $\Rightarrow~$ trigonometric functions appear
 - $\bullet~$ Improved actions $\Rightarrow~$ many additional operators contribute
 - $\bullet~$ No Lorentz symmetry $\Rightarrow~$ more complicated Lorentz index structures allowed
- Number of diagrams grows very quickly
 - Vertices of arbitrary adicity \Rightarrow many possible contractions from high-adicity vertices
 - Book-keeping effort grows rapidly
- Standard tricks don't work
 - $\bullet\,$ Trigonometric functions $\Rightarrow\,$ inverse propagator is not a quadratic form
 - $\bullet~$ No Lorentz symmetry \Rightarrow cannot use it to simplify numerators
 - Cannot complete squares; no Schwinger parameter representation; no Feynman trick

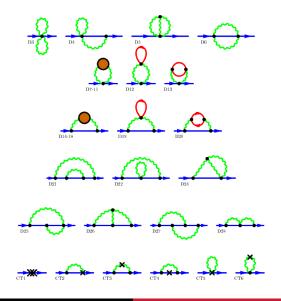
$$\begin{split} W^{abcd}_{\mu\nu\lambda\rho\rho}(p,q,r,s) &= -g_0^2 \Biggl\{ \sum_e f_{abe} f_{cde} \Biggl[\delta_{\mu\lambda} \delta_{\nu\rho} \Biggl(\cos \frac{a(q-s)_{\mu}}{2} \cos \frac{a(k-r)_{\nu}}{2} - \frac{a^4}{12} \widehat{k}_{\nu} \widehat{q}_{\mu} \widehat{r}_{\nu} \widehat{s}_{\mu} \Biggr) \\ &- \delta_{\mu\rho} \delta_{\nu\lambda} \Biggl(\cos \frac{a(q-r)_{\mu}}{2} \cos \frac{a(k-s)_{\nu}}{2} - \frac{a^4}{12} \widehat{k}_{\nu} \widehat{q}_{\mu} \widehat{r}_{\mu} \widehat{s}_{\nu} \Biggr) \Biggr\} \\ &+ \frac{1}{6} \delta_{\nu\lambda} \delta_{\nu\rho} a^2 (\widehat{s-r})_{\mu} \widehat{k}_{\nu} \cos \frac{aq_{\mu}}{2} - \frac{1}{6} \delta_{\mu\lambda} \delta_{\mu\rho} a^2 (\widehat{s-r})_{\nu} \widehat{q}_{\mu} \cos \frac{ak_{\nu}}{2} \\ &+ \frac{1}{6} \delta_{\mu\nu} \delta_{\mu\rho} a^2 (\widehat{q-k})_{\lambda} \widehat{r}_{\rho} \cos \frac{as_{\lambda}}{2} - \frac{1}{6} \delta_{\mu\nu} \delta_{\mu\lambda} a^2 (\widehat{q-k})_{\rho} \widehat{s}_{\lambda} \cos \frac{ar_{\rho}}{2} \\ &+ \frac{1}{12} \delta_{\mu\nu} \delta_{\mu\lambda} \delta_{\mu\rho} a^2 (\widehat{q-k})_{\sigma} (\widehat{s-r})_{\sigma} \Biggr] \\ &+ (b \leftrightarrow c, \nu \leftrightarrow \lambda, q \leftrightarrow r) + (b \leftrightarrow d, \nu \leftrightarrow \rho, q \leftrightarrow s) \Biggr\} \\ &+ \frac{g_0^2}{12} a^4 \Biggl\{ \frac{2}{3} (\delta_{ab} \delta_{cd} + \delta_{ac} \delta_{bd} + \delta_{ad} \delta_{bc}) + \sum_e (\delta_{abe} \delta_{cde} + \delta_{ace} \delta_{bde} + \delta_{ade} \delta_{bce}) \Biggr\} \\ &\times \Biggl\{ \delta_{\mu\nu} \delta_{\mu\lambda} \delta_{\mu\rho} \sum_{\sigma} \widehat{k}_{\sigma} \widehat{q}_{\sigma} \widehat{r}_{\sigma} \widehat{s}_{\sigma} - \delta_{\mu\nu} \delta_{\mu\lambda} \widehat{k}_{\rho} \widehat{q}_{\rho} \widehat{r}_{\rho} \widehat{s}_{\mu} \\ &- \delta_{\mu\nu} \delta_{\mu\rho} \widehat{k}_{\lambda} \widehat{q}_{\lambda} \widehat{s}_{\lambda} \widehat{r}_{\mu} - \delta_{\mu\lambda} \delta_{\mu\rho} \widehat{k}_{\nu} \widehat{r}_{\nu} \widehat{s}_{\mu} + \delta_{\mu\rho} \delta_{\nu\lambda} \widehat{k}_{\nu} \widehat{s}_{\mu} \widehat{q}_{\mu} \widehat{r}_{\mu} \Biggr\} \Biggr\} \end{split}$$

- This was the simplest possible gauge action (Wilson)!
- Improvement makes things much worse:

	# of terms for					
	prop.	3-gluon	4-gluon	5-gluon	6-gluon	
Wilson	76	240	826	1583	3184	
Symanzik	252	1456	6022	15488	36148	

• Quark actions become even worse after improvement:

	# of terms for					
	prop.	1-gluon	2-gluon	3-gluon		
Naive	9	8	8	8		
Asqtad	17	1248	8376	29480		
Fat3	9	152	2888	54584		
Fat5	9	632	49928	?		
Fat7	9	1080	145800	?		



G.M. von Hippel Automated Perturbation Theory

• The number of Feynman diagrams grows quickly:

	continuum	lattice
1-loop quark s.e.	1	2
1-loop gluon s.e.	4	7
1-loop qqg vertex corr.	2	6
1-loop ggg vertex corr.	8	16
2-loop quark s.e.	11	29

- If one wishes to simplify the numerator algebra on the lattice, the lack of Lorentz invariance makes the calculations much more involved.
- Ultimately, lattice integrals cannot be evaluated analytically, and have to be treated with numerical integration methods.

What can we do about it?

- Automate the derivation of the Feynman rules
 - Avoid human error in the extremely complex calculation
 - Enable use of highly improved actions, iterated smearing and higher orders
 - Algorithm easily implementable in any language with list and dictionary types (e.g. Python)
 - Output in machine-readable format for use by separate generic vertex code
- Automate the generation of the Feynman diagrams
 - Take advantage of generic vertex code
 - At least for low orders, we can simply apply Wick's theorem
- Automate the evaluation of the Feynman diagrams
 - Use numerical integration (e.g. VEGAS) or finite-volume sums
 - Employ techniques of automatic differentiation

• Lattice gauge action is given as a sum of Wilson loops:

$$S_g = \beta \sum_i c_i \sum_x \operatorname{Re} \operatorname{Tr} (U_{C_i}(x))$$

• We want the action in vertex form:

$$S_g = \sum_r \frac{g_0^{r-2}}{r!} \sum_{x, v_1, \dots, v_r} V_{\mu_1 \cdots \mu_r}^{\mathfrak{a}_1 \cdots \mathfrak{a}_r}(x, v_1, \dots, v_r) A_{\mu_1}^{\mathfrak{a}_1}(v_1) \cdots A_{\mu_r}^{\mathfrak{a}_r}(v_r)$$

• From this, the vertex functions in momentum space are obtained as

$$V^{a_1\cdots a_r}_{\mu_1\cdots \mu_r}(k_1,\ldots,k_r) = \operatorname{Tr}(t^{a_1}\cdots t^{a_r}) \\ \times \sum_i f_{\{\mu\},i} \mathrm{e}^{i\sum_j k_j\cdot \mathbf{v}_{\{\mu\},i,j\}}}$$

 Lattice fermion action is given as a sum of Wilson lines capped by fermion fields:

$$S_{f} = \sum_{i} c_{i} \sum_{x} \bar{\psi}(y_{i}) \Gamma_{i} U_{\mathcal{D}_{i}}(y_{i}, x) \psi(x)$$

• We want the action in vertex form:

$$S_{f} = \sum_{r} \frac{g_{0}^{r}}{r!} \sum_{y,x,v_{1},\ldots,v_{r}} \overline{\psi}^{b}(y) W_{\mu_{1}\cdots\mu_{r}}^{a_{1}\cdots a_{r},b^{c}}(x,y,v_{1},\ldots,v_{r}) A_{\mu_{1}}^{a_{1}}(v_{1})\cdots A_{\mu_{r}}^{a_{r}}(v_{r})\psi^{c}(x)$$

• From this, the fermionic vertex functions are obtained as

$$W^{a_1\cdots a_r,bc}_{\mu_1\cdots \mu_r}(k_1,\ldots,k_r;p,q) = (t^{a_1}\cdots t^{a_r})_{bc} \\ \times \sum_i f_{\{\mu\},i} \Gamma_{\alpha_{\{\mu\},i}} e^{i(p\cdot x_{\{\mu\},i}+q\cdot y_{\{\mu\},i}+\sum_j k_j\cdot v_{\{\mu\},i,j})}$$

- Need to automate translation [Lüscher, Weisz, NPB 266 (1986) 309; Hart, vH, Horgan, Müller, arXiv:0904.0375] {(c, Γ, C)} → {({µ}, {v}, y, Γ, f)}
- The basic object is a gauge link

$$U_{\mu}(x) = e^{ig_{\theta}A_{\mu}(x+\frac{1}{2}\hat{\mu})} = \sum_{r=0}^{\infty} \frac{g^{r}}{r!} t^{a_{1}} \cdots t^{a_{r}} A_{\mu}^{a_{1}}(x+\frac{1}{2}\hat{\mu}) \cdots A_{\mu}^{a_{r}}(x+\frac{1}{2}\hat{\mu})$$

Hence, basic mapping is

$$F(U_{\mu}) = \{(\mu; \frac{1}{2}\hat{\mu}; \hat{\mu}; \mathbb{1}; 1), (\mu, \mu; \frac{1}{2}\hat{\mu}, \frac{1}{2}\hat{\mu}; \hat{\mu}; \mathbb{1}; 1), \ldots\}$$

Build action from links by using

$$F(U_{\mathcal{C}} + U_{\mathcal{C}'}) = F(U_{\mathcal{C}}) \cup F(U_{\mathcal{C}'})$$

$$F(cU_{\mathcal{C}}) = \{cE : E \in F(U_{\mathcal{C}})\}$$

$$F(\Gamma U_{\mathcal{C}}) = \{\Gamma E : E \in F(U_{\mathcal{C}})\}$$

$$F(U_{\mathcal{C}}U_{\mathcal{C}'}) = \{E * E' : E \in F(U_{\mathcal{C}}), E' \in F(U_{\mathcal{C}'})\}$$

• We need algebra of expansion entities $E = (\{\mu\}; \{\nu\}; y; \Gamma; f)$:

$$cE = (\{\mu\}; \{\nu\}; y; \Gamma; cf)$$

$$\Gamma'E = ((\{\mu\}; \{\nu\}; y; \Gamma'\Gamma; f))$$

$$E * E' = (\{\mu\} \cup \{\mu'\}; \{\nu\} \cup \{\nu' + y\}; y' + y; \Gamma\Gamma'; Cff')$$

- In practice, naive implementation of link algebra in terms of entity algebra will yield many redundant entities
- To avoid associated cost, implement link algebra in terms of dictionaries mapping partial entities Ê = ({μ}; {v}; γ; Γ) to their associated amplitude f
- Momentum conservation means that ({μ}; {v}; γ; Γ) and ({μ}; {v + c}; y + c; Γ) give same contribution to vertex
- Identify and combine entities that differ only by a constant translation of their vectors



- The resulting expansion of the action in terms of entities is written out in a machine-readable format
- The HPSRC library of generic vertex functions vertex_*(k,mu,a) is used to construct Feynman diagrams
- The HPSRC library reads in the list of entities at runtime and constructs vertices from entities on the fly
- This separates the coding of the Feynman diagrams from the derivation of the Feynman rules
- Note that this allows to rerun a calculation with a different action with as little overhead as possible
- For very complex actions, the HPSRC library allows to factor the action into parts whose Feynman rules are derived separately and combined on the fly at runtime
- Also includes hand-written Feynman rules for Fadeev-Popov ghosts and for counterterms from the Haar measure

Automating the generation of lattice Feynman diagrams

- Feynman diagrams can be generated by applying Wick's theorem
- For one-loop calculations, it is generally easier to code the diagrams by hand
- For two-loop calculations, a straightforward implementation of Wick's theorem is currently used
- Standard tools like QGRAF could be used, but these would need adapting for Lattice QCD
- It is extremely desirable to output the diagrams directly as sequences of function calls to the HPSRC generic vertex routines
- Further work needed in this area if one wants to go to even higher orders

Automating the evaluation of lattice Feynman diagrams

- For the numerical evaluation of the lattice integrals we use parallel VEGAS (for lattices with infinite extent) or trivially parallelised finite-volume mode sums (for finite lattices)
- We usually need wavefunction renormalisation constants, i.e. derivatives of self-energy diagrams
- Require methods of automatic differentiations [vH, arXiv:0910.5111]
- Implement a type that encodes a function along with its first few derivatives w.r.t. external momentum
- Overload arithmetic operations to fulfill Leibniz's and Faà di Bruno's rules



$$\frac{d^{n}}{dx^{n}}(fg)(x) = \sum_{k=0}^{n} \binom{n}{k} f^{k}(x) g^{(n-k)}(x)$$
$$\frac{d^{n}}{dx^{n}} f(g(x)) = \sum_{\substack{\mathbf{0} \le k_{\mu} \le n \\ \sum_{\mu} \mu^{k} \mu = n}} \frac{n!}{\prod_{\nu} k_{\nu}! \nu!^{k_{\nu}}} \frac{d^{|k|} f}{dy^{|k|}} \prod_{\mu=1}^{n} \left(\frac{d^{\mu}g}{dx^{\mu}}\right)^{k_{\mu}}$$



- Derivatives of vertex functions are simple to compute (exponentials!)
- Overloaded operations take care of the rest

Applications

- Unquenching contributions from improved staggered quarks
 - asqtad [Hao, vH, Horgan, Mason, Trottier, arXiv:0705.4660]
 - HISQ [Hart, vH, Horgan, arXiv:0812.0503]
- Improving the NRQCD action
 - hyperfine splittings [Hammant, Hart, vH, Horgan, Monahan, arXiv:1105.5309, arXiv:1303.3234]
 - kinetic couplings [Davier, Harrison, Hughes, Horgan, vH, Wingate, arXiv:1812.11639]
 - hindered M1 radiative decays of ↑(2S) [Hughes, Dowdall, Davies, Horgan, vH, Wingate, arXiv:1508.01694]
 - leptonic widths of S-wave quarkonia [Hart, vH, Horgan, hep-lat/0605007]
- Perturbative subtraction of lattice artifacts in NPR
 - with Wilson quarks [Harris, vH, Junnarkar, Meyer, Ottnad, Wilhelm, Wittig, Wrang, arXiv:1905.01291]

Did you say staggered?

- Actually, the staggered calculations were done with naive fermions.
- But this is essentially the same thing (except easier):
 - The naive propagator is

$$S(x,y) = g(x,y)\Omega(x)\Omega(y)^{\dagger}$$

in terms of the single-component staggered propagator \boldsymbol{g} and the Kawamoto-Smit transform

$$\Omega(x) = \prod_{\mu} (\gamma_{\mu})^{\frac{x_{\mu}}{a}}$$

• whence the vertices become

$$\Omega(x+\hat{\mu})^{\dagger}\Gamma_{\mu}\Omega(x) = \alpha_{\mu}(x)\mathbb{1}$$

in terms of staggered phase factors

$$\alpha_{\mu}(x) = (-1)^{\sum_{\nu < \mu} \frac{x_{\nu}}{a}}$$

- This implies that
 - naive loops are four times the corresponding staggered loop,
 - naive incoming (outgoing) legs give a factor Ω (Ω^{\dagger}),
 - everything else just goes through.

- There is actually a version of Reisz's power-counting theorem for staggered fermions [Giedt, hep-lat/0606003]
- No completed proof of perturbative renormalizability, though
- But no reason to expect serious obstacles

- No direct technical obstacles to applying automated methods
- Four-component spinors, Wilson-like structure (naive + symmetry-breaking)
- Breaking of discrete spacetime symmetries not a problem in automated treatment
- Taste structure may require some interpreting, though