Automated Lattice Perturbation Theory in the Schrödinger Functional and HQET Flavor Currents

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Thanks to: P. Fritzsch, N. Garron, G.M. von Hippel, M. Kurth, H. Simma, S. Takeda, U. Wolff

Beautiful Mesons and Baryons on the Lattice, Trento, April 2012

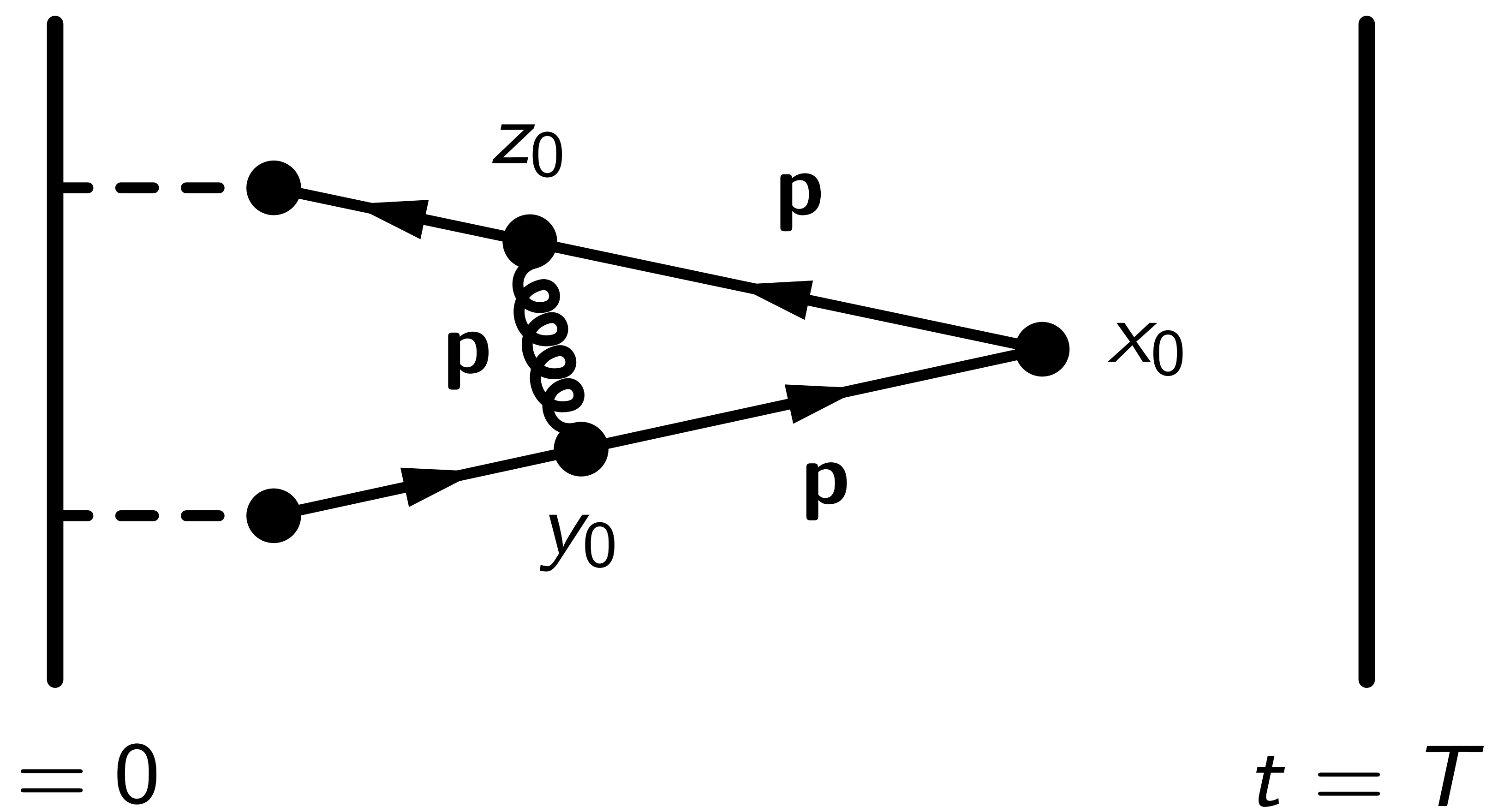
Outline

- Theory: How to/why automate LPT?!
- How ALPT can help with the HQET matching!

Automation?!

We want to evaluate expressions like this one:

$$\sum_{\mathbf{p},y_0,z_0} \mathrm{tr} \left\{ \quad \right\}$$

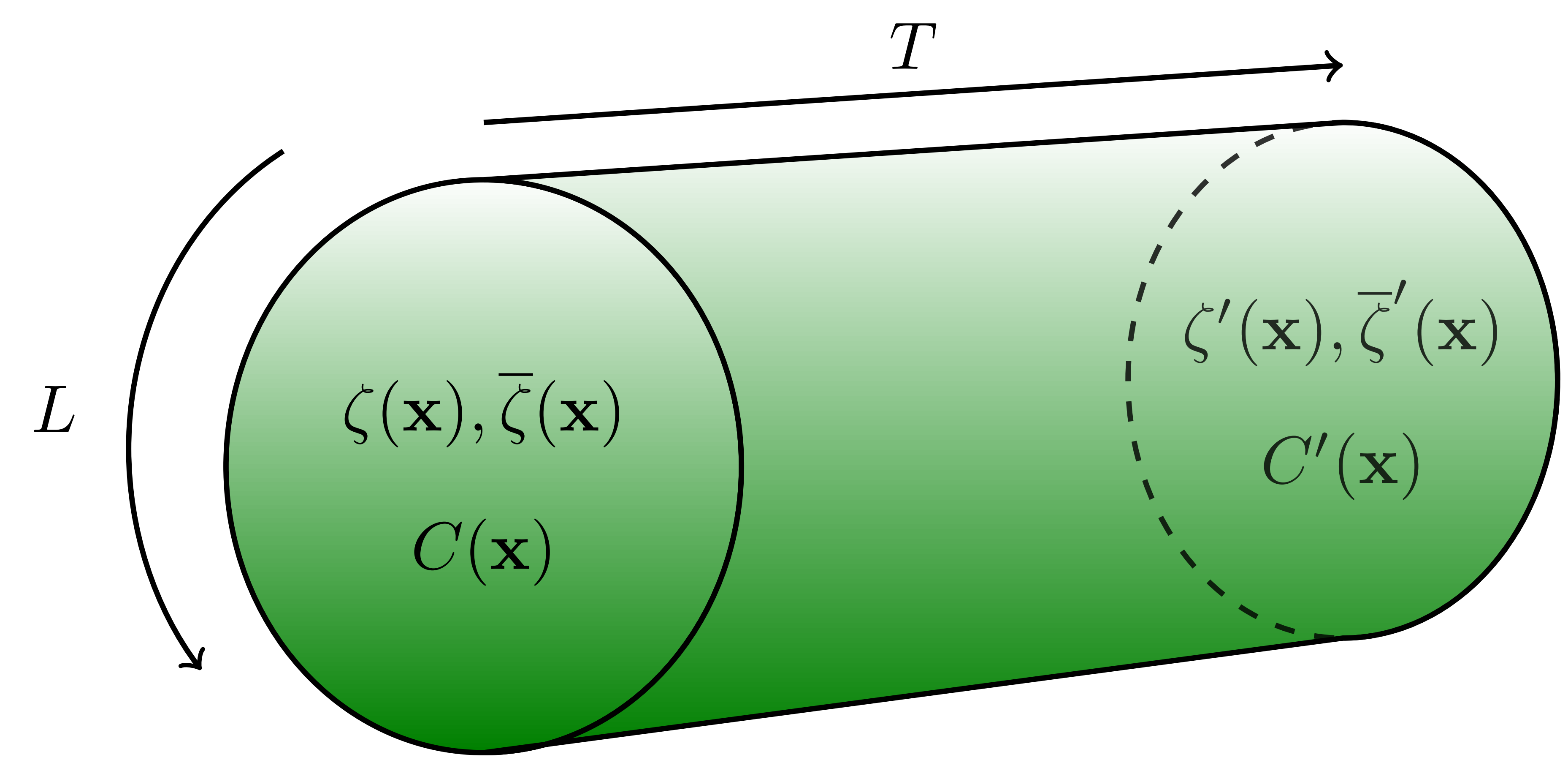


With *automation* I mean automatic generation of

Feynman diagrams **and**

Feynman rules!

The Schrödinger Functional



$$\zeta(\mathbf{x}) = \sum_y \tilde{K}(\mathbf{x}, y)\psi(y), \quad \zeta'(\mathbf{x}) = \sum_y \tilde{K}'(\mathbf{x}, y)\psi(y),$$

$$\overline{\zeta}(\mathbf{x}) = \sum_y \psi(y)K(y, \mathbf{x}), \quad \overline{\zeta}'(\mathbf{x}) = \sum_y \psi(y)K'(y, \mathbf{x}),$$

$$P_+\psi(x)|_{x_0=0} = \overline{\psi}(x)P_-|_{x_0=0} = 0$$

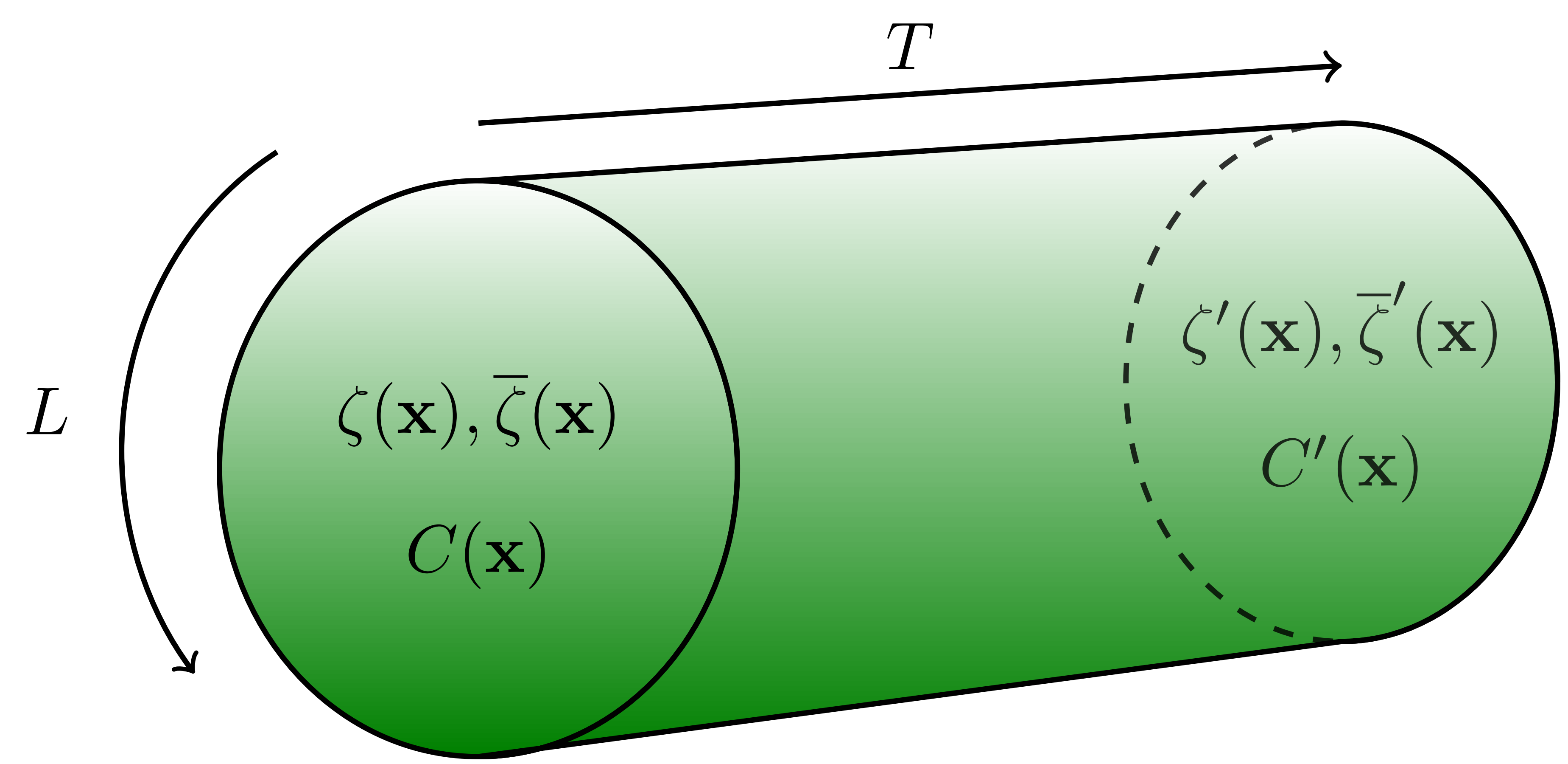
$$P_-\psi(x)|_{x_0=T} = \overline{\psi}(x)P_+|_{x_0=T} = 0,$$

$$P_\pm = 1/2(1 \pm \gamma_0)$$

$$\psi(x + L\,\hat{k}) = e^{i\theta_k}\psi(x).$$

M. Lüscher, P. Weisz, R. Narayanan, U. Wolff, 1992. S. Sint, 1996, M. Lüscher 2006.

The Schrödinger Functional



$$U_\mu(x + \hat{k}L) = U_\mu(x),$$

$$U_k(x)|_{x_0=0} = e^{C(\mathbf{x})}, \quad U_k(x)|_{x_0=T} = e^{C'(\mathbf{x})}.$$

This induces a background field,

$$U_\mu(x) = \exp\{g_0 q_\mu(x)\} V_\mu(x).$$

M. Lüscher, P. Weisz, R. Narayanan, U. Wolff, 1992. S. Sint, 1996, M. Lüscher 2006.

Diagram Generation

For example, take $\mathcal{O} = \overline{\psi}_1(x)\,\gamma_0\gamma_5\,\psi_2(x)\,\overline{\zeta}_2(\mathbf{y})\,\gamma_5\,\zeta_1(\mathbf{z})$.

Split up gauge and fermion averages, $\langle \mathcal{O} \rangle = \langle [\mathcal{O}]_F \rangle_G$.

First perform fermion Wick contractions,

$$\langle \mathcal{O} \rangle = \langle\, \overline{\psi}_1(x)\,\gamma_5\,\psi_2(x)\,\overline{\zeta}_2(\mathbf{y})\,\gamma_5\,\zeta_1(\mathbf{z})\,\rangle_G$$

$$= \langle\, [\zeta_1(\mathbf{z})\overline{\psi}_1(x)]_F\,\gamma_5\,[\psi_2(x)\overline{\zeta}_2(\mathbf{y})]_F\,\gamma_5\,\rangle_G.$$

Then the gauge average,

$$\langle f \rangle_G = \frac{1}{Z}\int \mathcal{D}[U] e^{-S_G[U]}\mathcal{Z}_F[U] f[U],$$

$$\mathcal{Z}_F[U] = \int \mathcal{D}[\overline{\psi},\psi] e^{-S_F[\overline{\psi},\psi,U]}.$$

Fermion Wick Contractions

Key observation:

All basic fermion Wick contractions may be written in terms of the **propagator** $S = (D+m)^{-1}$ (for a given gauge field) and the **boundary kernels** $K, K', \ldots$

Where
$$\frac{\delta}{\delta\overline{\psi}(x)} S_F = (D+m)\psi(x), \quad 0 < x_0 < T.$$

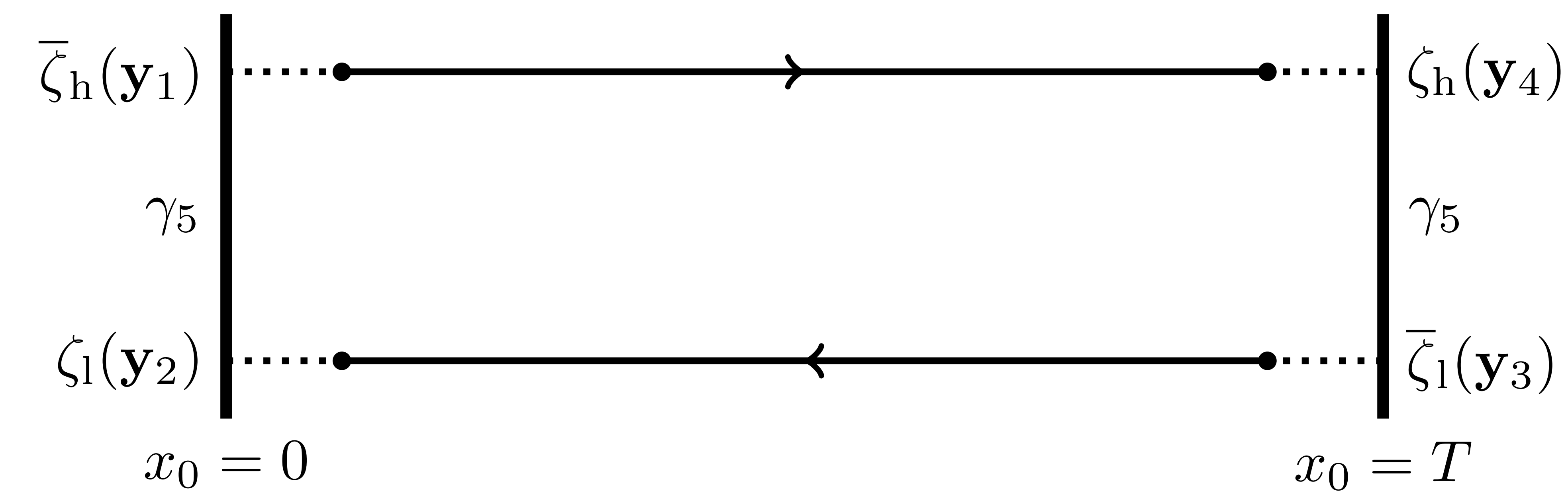
For example
$$[\psi(x)\overline{\psi}(y)]_F = S(x,y),$$
$$[\psi(x)\overline{\zeta}(\mathbf{z})]_F = \sum_y S(x,y)\,K(y,\mathbf{z}).$$

M. Lüscher, P. Weisz, 1996.

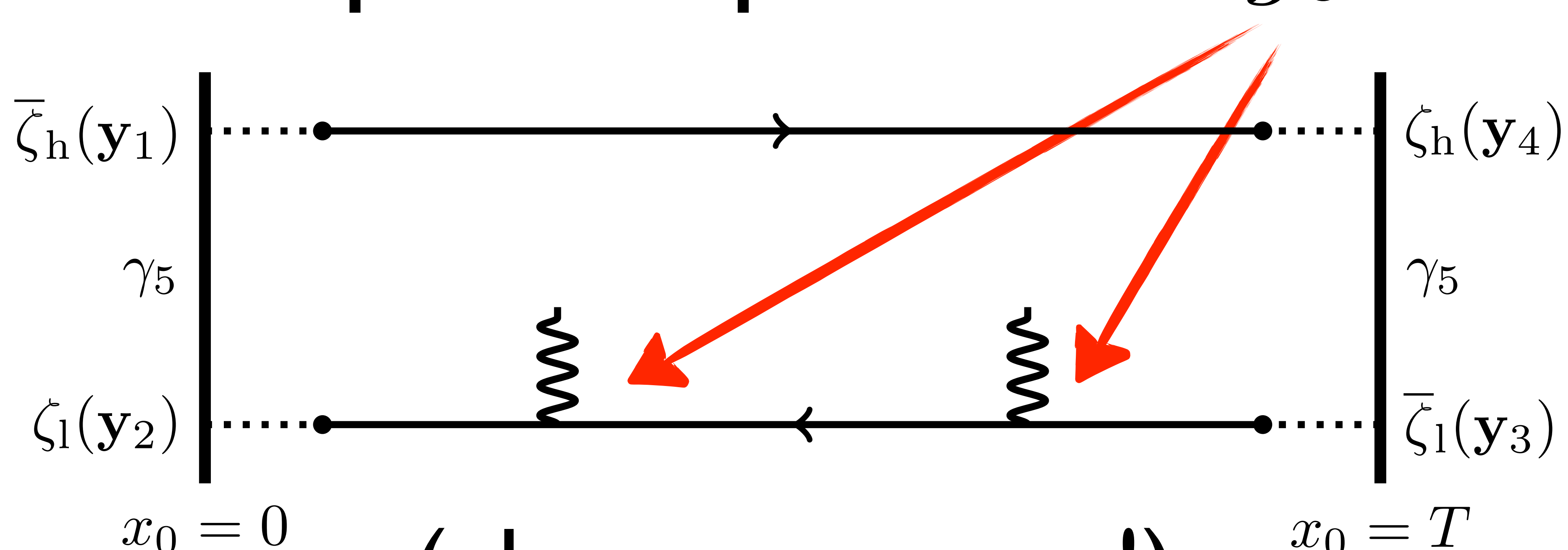
ALPT - The Comic

Your favorite observable

Fermion Wick contractions

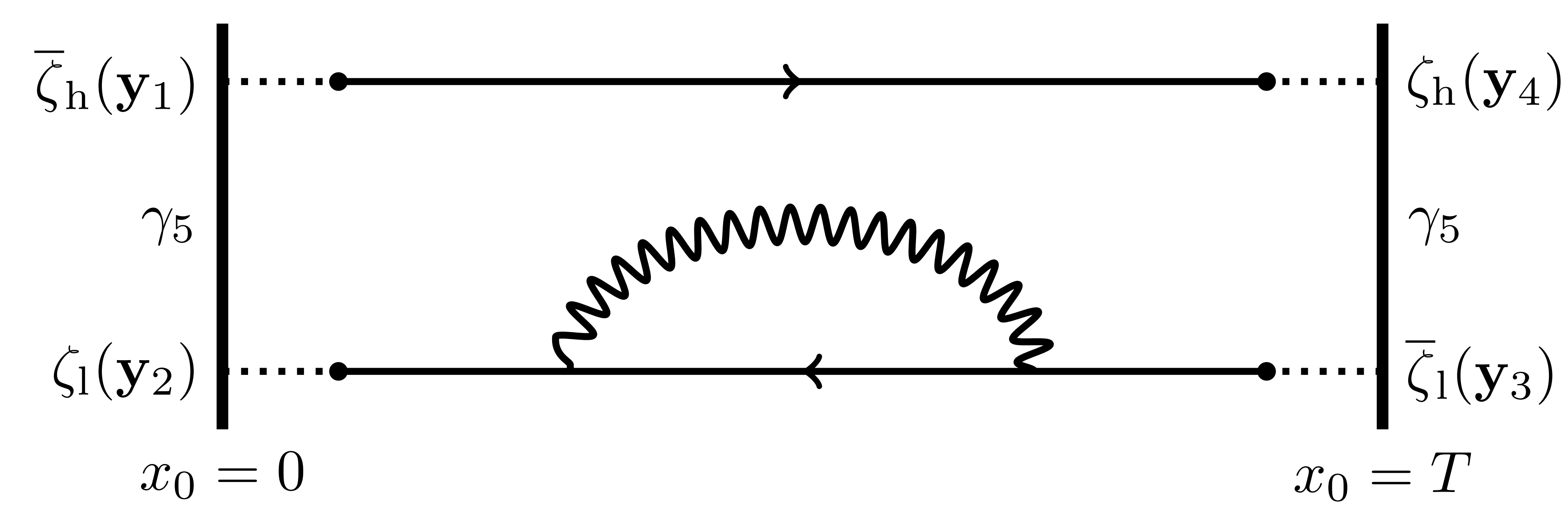


Expand in powers of g_0



(plus many more!)

Gluon Wick contractions



Perturbative Expansion

Now, expand

$$S(x,y) = S^{(0)}(x,y) + g_0 S^{(1)}(x,y) + \dots$$
$$K(x,\mathbf{y}) = K^{(0)}(x,\mathbf{y}) + g_0 K^{(1)}(x,\mathbf{y}) + \dots$$

and perform the gluon Wick contractions.

We may obtain $S^{(i)}(x,y)$ by solving

$$\Big(D^{(0)} + m + g_0 D^{(1)} + \dots\Big)\Big(S^{(0)}(x,y) + g_0 S^{(1)}(x,y) + \dots\Big) = \delta_{xy}$$

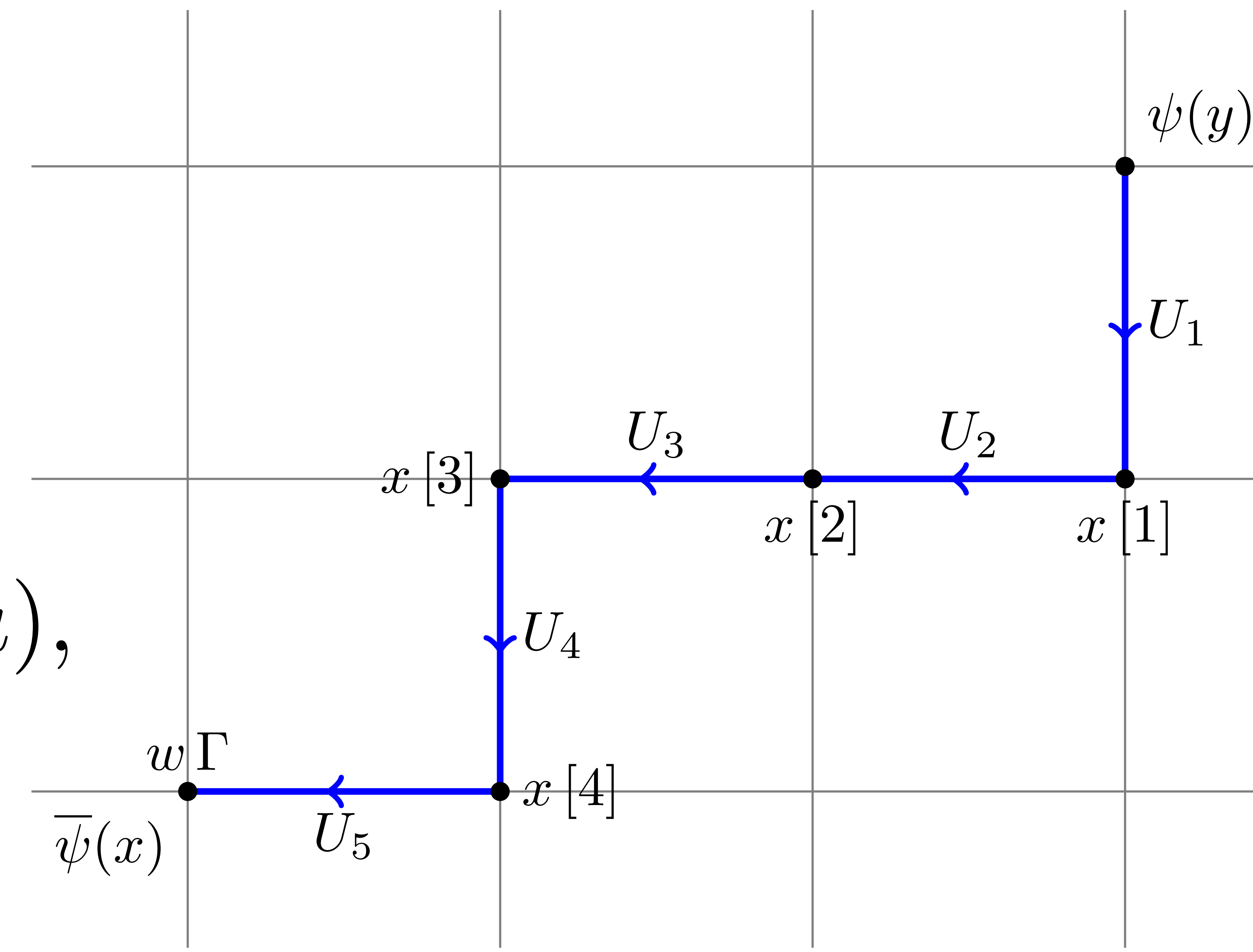
order by order.

M. Lüscher, P. Weisz, 1996.

Fermion Actions

We assume that the fermion action looks like this

$$
\begin{aligned}
S_F &= \sum_i c_i \,\overline{\psi}(x_i)\,\Gamma_i \mathcal{U}_i(x_i, y_i)\,\psi(y_i), \\
\mathcal{U}(x,y) &= U_l U_{l-1} \dots U_1, \\
U_i &= U_{s[i]\mu[i]}(x[i]), \quad U_{-\mu}(x) = U_\mu^\dagger(x-\hat{\mu}), \\
s[i]\,\hat{\mu}[i] &= x[i-1] - x[i], \quad x[0] = y.
\end{aligned}
$$



For a given parallel transporter $\mathcal{U}(x,y)$

the points $x[i]$ define a path $y \to x$.

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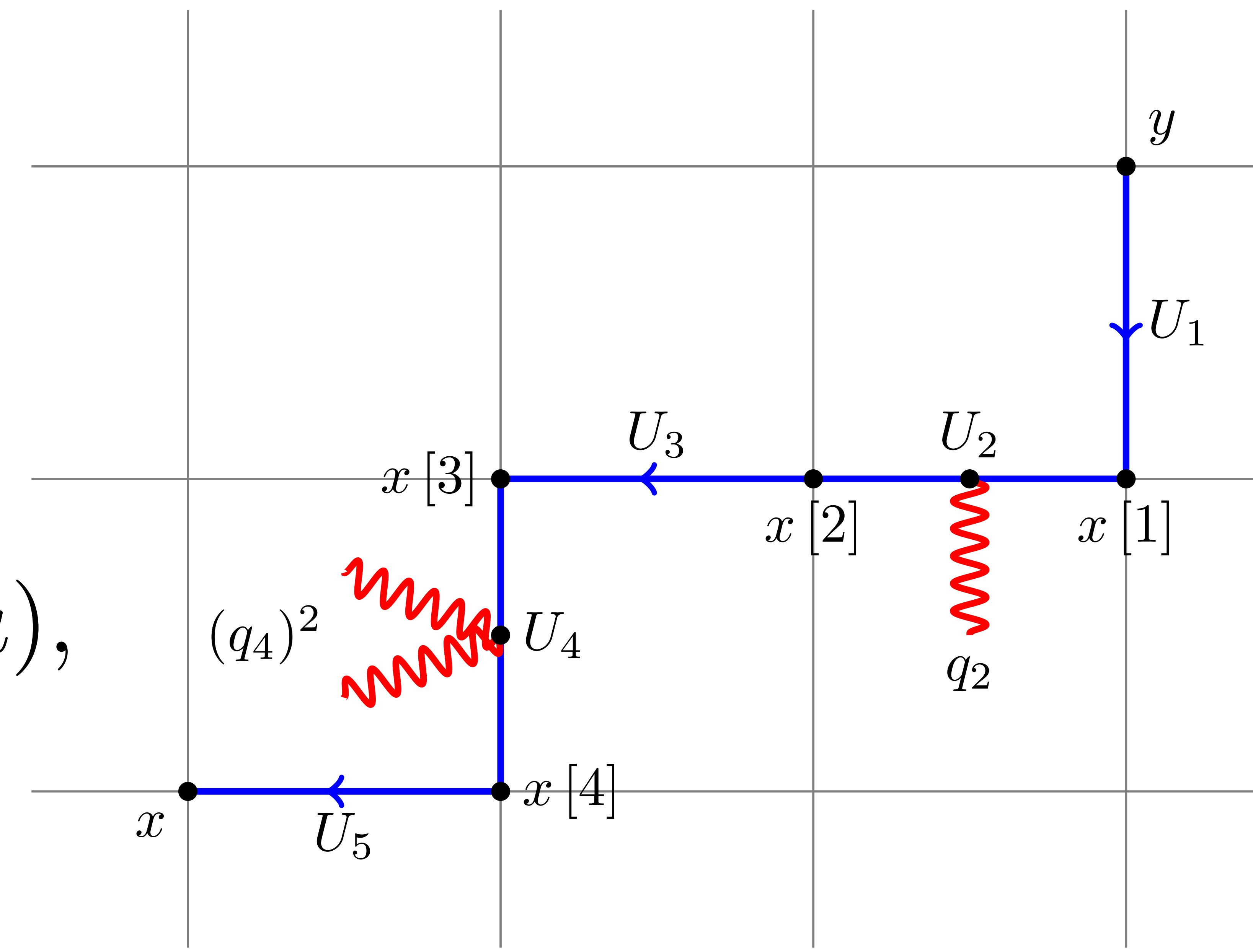

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Parallel Transporters

Each link as a simple expansion,

$$U_\mu(x) = \exp\{g_0\, q_\mu(x)\} V_\mu(x).$$

... but the whole parallel transporter has not...

$$\mathcal{U}(x,y) = \sum_r \frac{g_0^r}{r!}\,\mathcal{U}^{(r)}(x,y) = \sum_{n_l} \frac{g_0^{n_l}}{n_l!}\; q_l^{n_l}\; V_l \ldots \sum_{n_1} \frac{g_0^{n_1}}{n_1!}\; q_1^{n_1} V_1 .$$

General strategy:

Bring the contributions to a standard form.
Define a multiplication rule and construct $\mathcal{U}^{(r)}$ link by link.

M. Lüscher, P. Weisz, 1986. A. Hart, G.M. von Hippel, et. al., 2009. S. Takeda, U. Wolff, 2007.

pastor

User input:

- Fermion and gluon action in symbolic form.
- Observables in terms of propagators and boundary kernels.

Output:

All contributions (including $O(a)$ improvement) up to $O(g_0^2)$.

The basic steps are

1) Create a XML input file.
2) Parse the file to generate C++ programs.
3) Run the programs.

Data Analysis

An observable with at most a logarithmic divergence looks like this

$$f(I) = \sum_{n=0}^{\infty} \frac{a_n + b_n \log I}{I^n} \qquad I = L/a$$

M. Lüscher, P. Weisz, 1996.

We extract the coefficients using successive fits.

A. Bode, P. Weisz, U. Wolff, 2000.

Round-off errors can be estimated using `long double` precision.

Using pastor as an Aid for the Matching of HQET and QCD

Flavor Currents

$$\left(V_{\mathrm{R}}^{\mathrm{HQET}}\right)_0(x) = Z_{\mathrm{V}}^{\mathrm{HQET}}\left[V_0^{\mathrm{stat}} + \sum_{i=1}^{2} c_{\mathrm{V}}^{(i)} V_0^{(i)}(x)\right], \quad \left(V_{\mathrm{R}}^{\mathrm{HQET}}\right)_k(x) = Z_{\mathbf{V}}^{\mathrm{HQET}}\left[V_k^{\mathrm{stat}} + \sum_{i=3}^{6} c_{\mathrm{V}}^{(i)} V_k^{(i)}(x)\right],$$

$$V_0^{\mathrm{stat}}(x) = \overline{\psi}_{\mathrm{l}}(x)\gamma_0\psi_{\mathrm{h}}(x),$$

$$V_0^{(1)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\gamma_i\left(\nabla_i^S - \overleftarrow{\nabla}_i^S\right)\psi_{\mathrm{h}}(x),$$

$$V_0^{(2)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\gamma_i\left(\nabla_i^S + \overleftarrow{\nabla}_i^S\right)\psi_{\mathrm{h}}(x)$$

$$V_k^{(3)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\gamma_k\gamma_i\left(\nabla_i^S - \overleftarrow{\nabla}_i^S\right)\psi_{\mathrm{h}}(x),$$

$$V_k^{(4)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\left(\nabla_k^S - \overleftarrow{\nabla}_k^S\right)\psi_{\mathrm{h}}(x),$$

$$V_k^{(5)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\gamma_k\gamma_i\left(\nabla_i^S + \overleftarrow{\nabla}_i^S\right)\psi_{\mathrm{h}}(x),$$

$$V_k^{(6)}(x) = \overline{\psi}_{\mathrm{l}}(x)\frac{1}{2}\left(\nabla_k^S + \overleftarrow{\nabla}_k^S\right)\psi_{\mathrm{h}}(x)$$

... and for the axial vector current ...

$$Z_{\mathbf{A}}^{\mathrm{HQET}}, Z_{\mathrm{A}}^{\mathrm{HQET}}, c_{\mathrm{A}}^{(i)}$$

In total16 matching coefficients for the currents (plus 3 in the action)!

Good Matching Conditions

With correctly matched parameters, we expect

$$X^{\mathrm{QCD}}(m_{\mathrm{h}}) = X^{\mathrm{stat}} + O(1/m_{\mathrm{h}}),$$

$$X^{\mathrm{QCD}}(m_{\mathrm{h}}) = X^{\mathrm{stat}} + c_{\mathrm{X}} X^{1/m_{\mathrm{h}}} + \omega_{\mathrm{kin}} X^{\mathrm{kin}} + \omega_{\mathrm{spin}} X^{\mathrm{spin}} + O(1/m_{\mathrm{h}}^2).$$

How big are the corrections really?

Very important question if we want to use X in a matching condition!

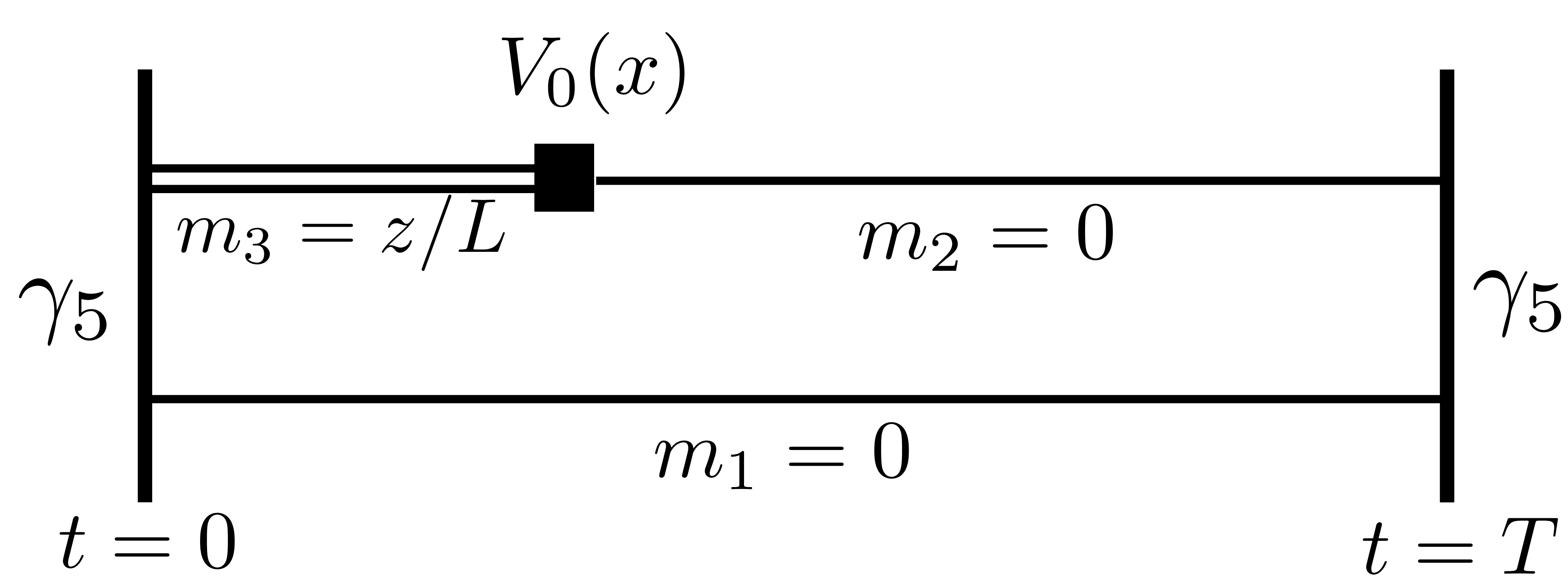
Matching the Vector Current

We define

$$f_1^{\mathrm{V}_0}(x_0;\theta,z=Lm_3) = -\frac{1}{2}\sum_{\mathbf{x}}\langle\overline{\zeta}_1\,\gamma_5\,\zeta_3\,V_0(x)\,\overline{\zeta}'_2\,\gamma_5\,\zeta'_1\rangle,$$

$$V_\mu(x) = \overline{\psi}_3(x)\gamma_\mu\psi_2(x), \quad \zeta_i = L^{-3/2}\sum_x \zeta_i(\mathbf{x})$$

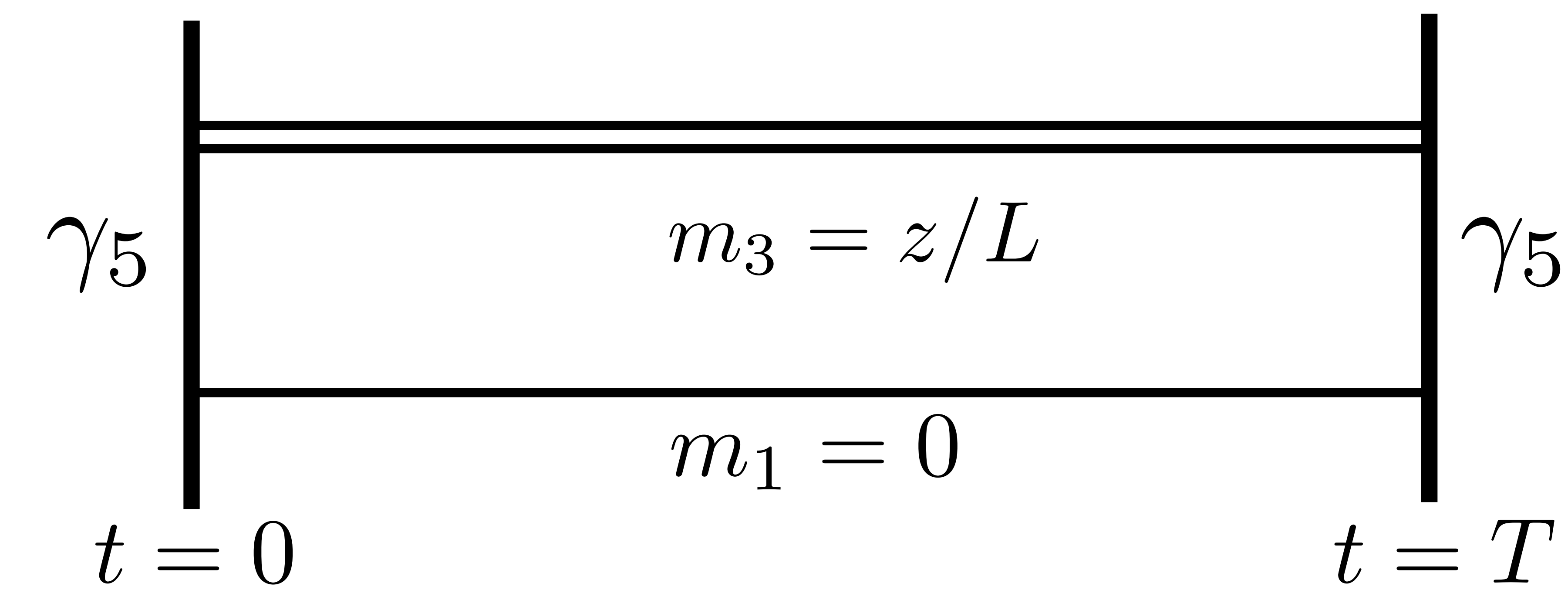
which looks like this:



The Full Observable

We also need the boundary-to-boundary correlator

$$f_1(\theta, z) = -\langle \overline{\zeta}_2'\, \gamma_5\, \zeta_3'\, \overline{\zeta}_3\, \gamma_5\, \zeta_2 \rangle$$



Lüscher, Sint, Sommer, and Weisz, *Nucl.Phys.*, B478:365– 400, 1996.

to construct

$$\Phi^{V_0}(\theta, z) = Z_V \frac{f_1^{V_0}(T/2; \theta, z)}{\sqrt{f_1(\theta, z) f_1(\theta, 0)}}.$$

Question: Is this a *good* observable for the matching?

The Static Approximation

We define

$$X_{\rm V}(\mu) = Z^{\rm stat}_{\rm A,lat}(\mu)\, Z^{\rm stat}_{\rm V/A} X^{\rm bare}_{\rm V}, \quad X^{\rm bare}_{\rm V} = \frac{\left(f_1^{\rm V_0}\right)^{\rm stat}(T/2;\theta)}{\sqrt{f_1^{\rm stat}(\theta) f_1(\theta,0)}},$$

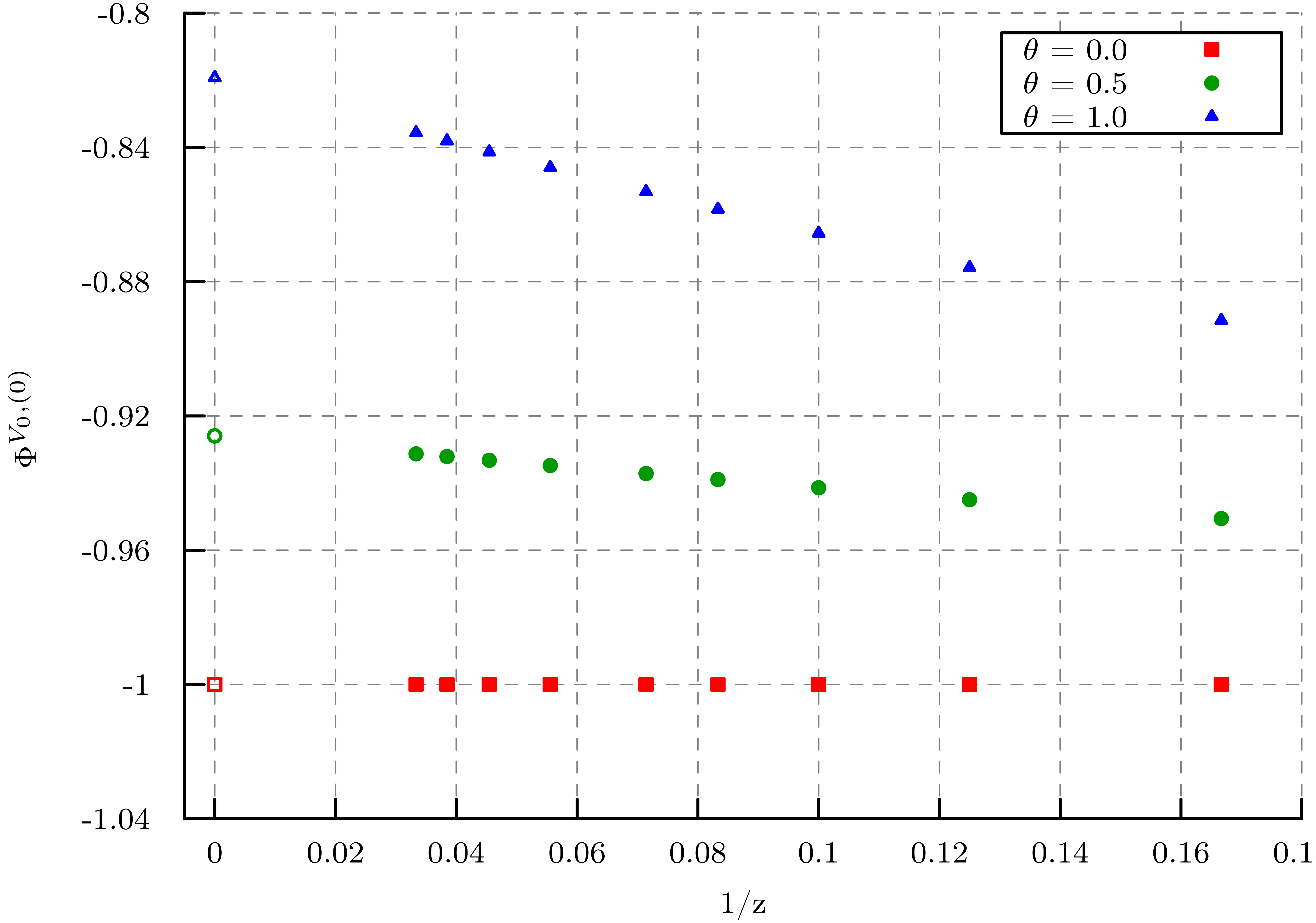
$$Z^{\rm stat}_{\rm A,lat}(\mu) = 1 - \gamma_0 \log(a\mu)\, g_0^2 + O(g_0^4).$$

One may then expect that up to **one loop**

$$\Phi^{\rm V_0}(z) = (1 + B^{\rm stat}_{\rm A} g_0^2) X_{\rm V}(z/L) + O(1/z).$$

M. Kurth, R. Sommer, 2001.

Tree Level



-0.8
-0.84
-0.88
-0.92
-0.96
-1
-1.04
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
$\Phi^{V_0,(0)}$
$1/z$
$\theta = 0.0$
$\theta = 0.5$
$\theta = 1.0$

One Loop - Theory

We define the quantity

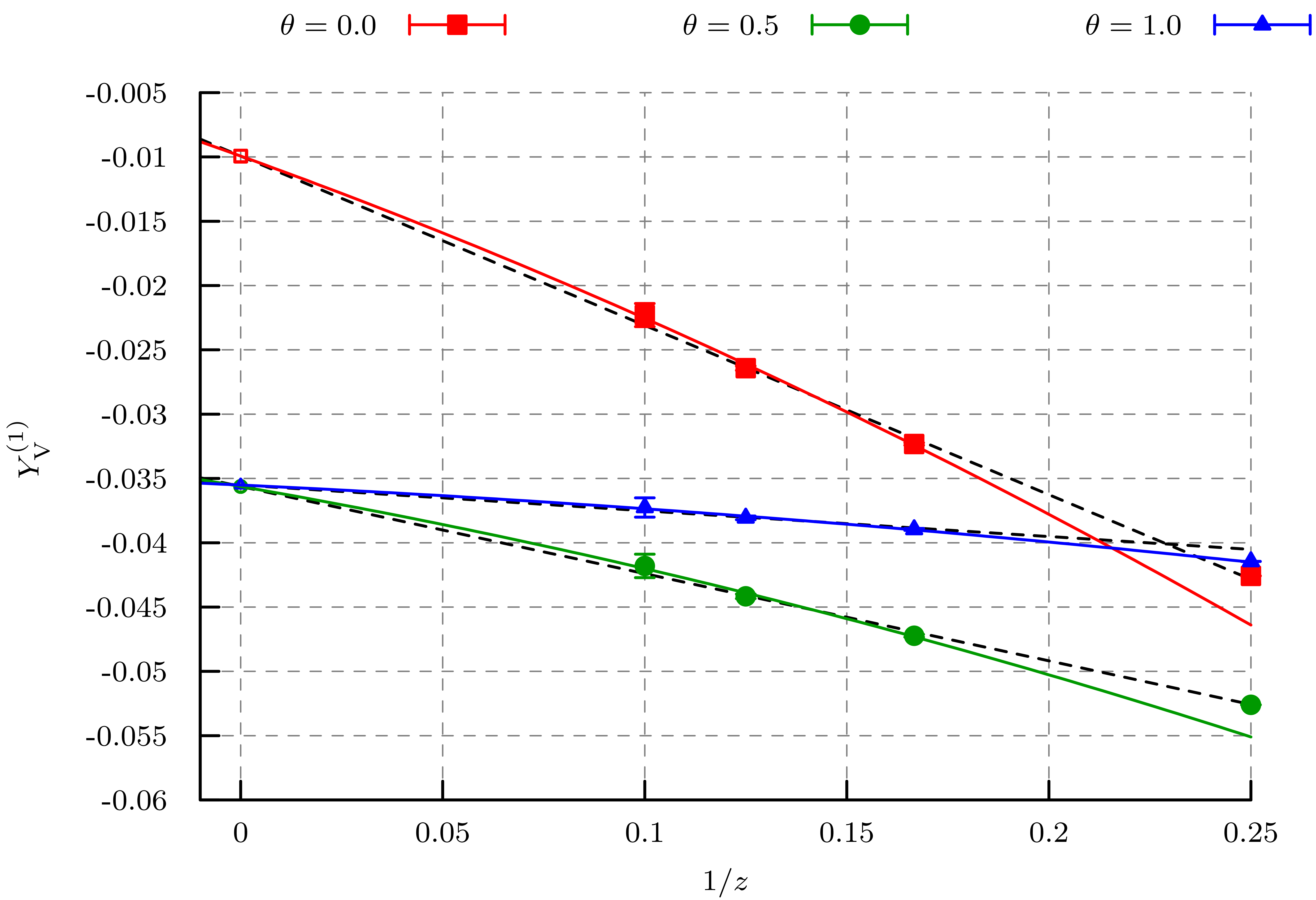
$$Y_{\mathrm{V}}^{(1)} = \Phi^{\mathrm{V}_0,(1)}(z) - \left[B_{\mathrm{V}}^{\mathrm{stat}} - \gamma_0 \log(z) + \left(Z_{\mathrm{V/A}}^{\mathrm{stat}} \right)^{(1)} \right] X_{\mathrm{V}}^{(0)},$$

and may expect that

$$Y_{\mathrm{V}}^{(1)}(z) \xrightarrow{1/z \to 0} X_{\mathrm{V,lat}}^{(1)} = X_{\mathrm{V}}^{\mathrm{bare},(1)} - \gamma_0 \log(a/L) X_{\mathrm{V}}^{\mathrm{bare},(0)}.$$

("lat" = lattice minimal subtraction)

One Loop - Results



The fit functions have the form

$$Y_{\mathrm{V}}^{(1)}(z) = X_{\mathrm{V,lat}}^{(1)} + c_1/z + c_2/z^2.$$

Very small $1/z, 1/z^2$ corrections (note the scale)!

Performance

Diagram count

	QCD	static
$f_1^{\mathrm{V}_0}$	30	29
f_1	22	21

Three values for θ

L/a = 4,...,40

Four values for z

Total time (incl. idle) on DESY PC farm in Zeuthen: Two weeks.

Conclusions/Outlook

- Improve pastor.
  - Better support for Abelian background.
  - Smearing.
  - Staggered quarks.
  - Chirally twisted boundary conditions.
  - Two loops?!
- More applications.
  - One loop matching of all components of the currents

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Appendix

Definitions

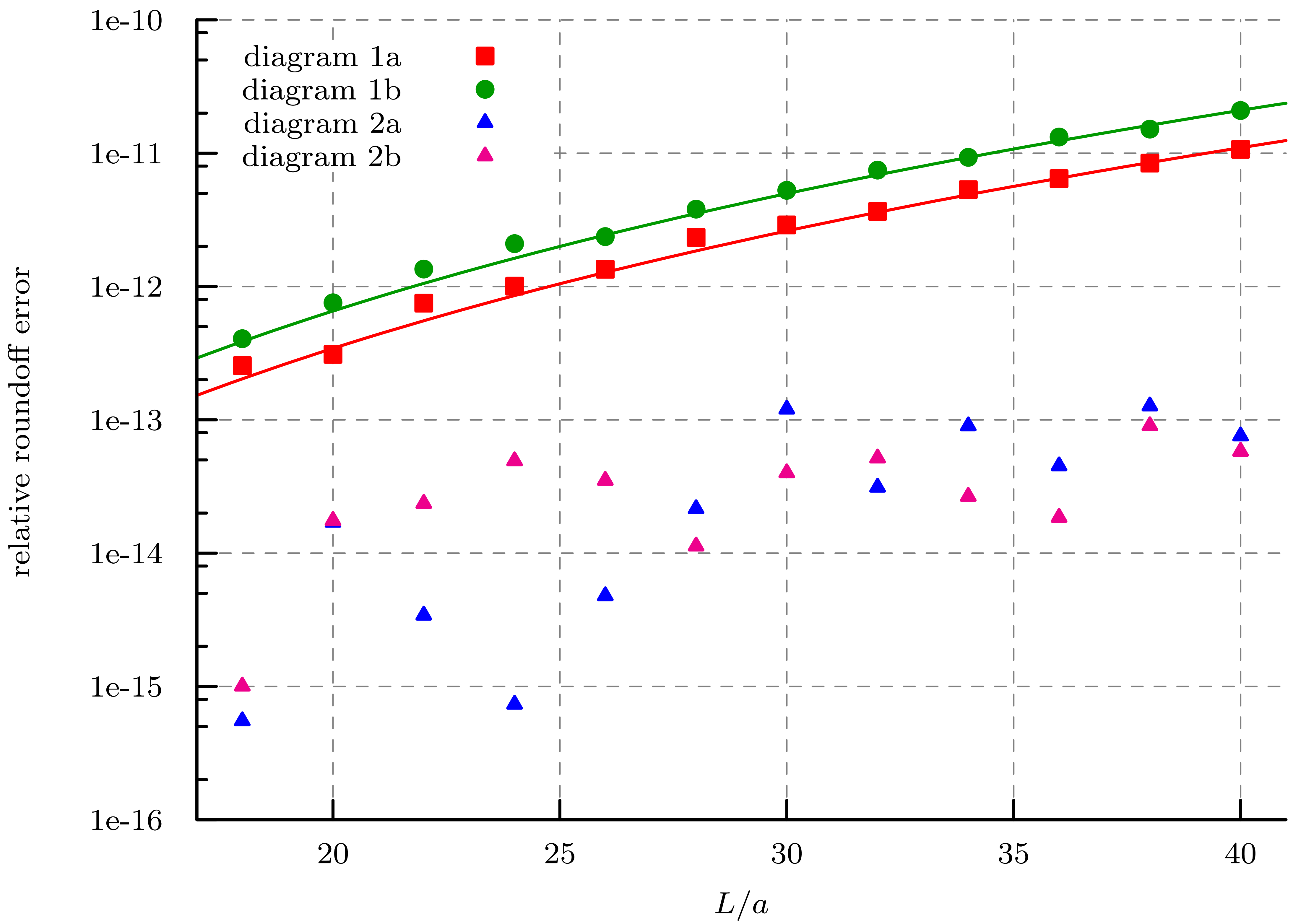
$$\mathcal{O}_{\rm kin}(x) = \overline{\psi}_{\rm h}(x)\nabla_k^*\nabla_k\psi_{\rm h}(x),$$

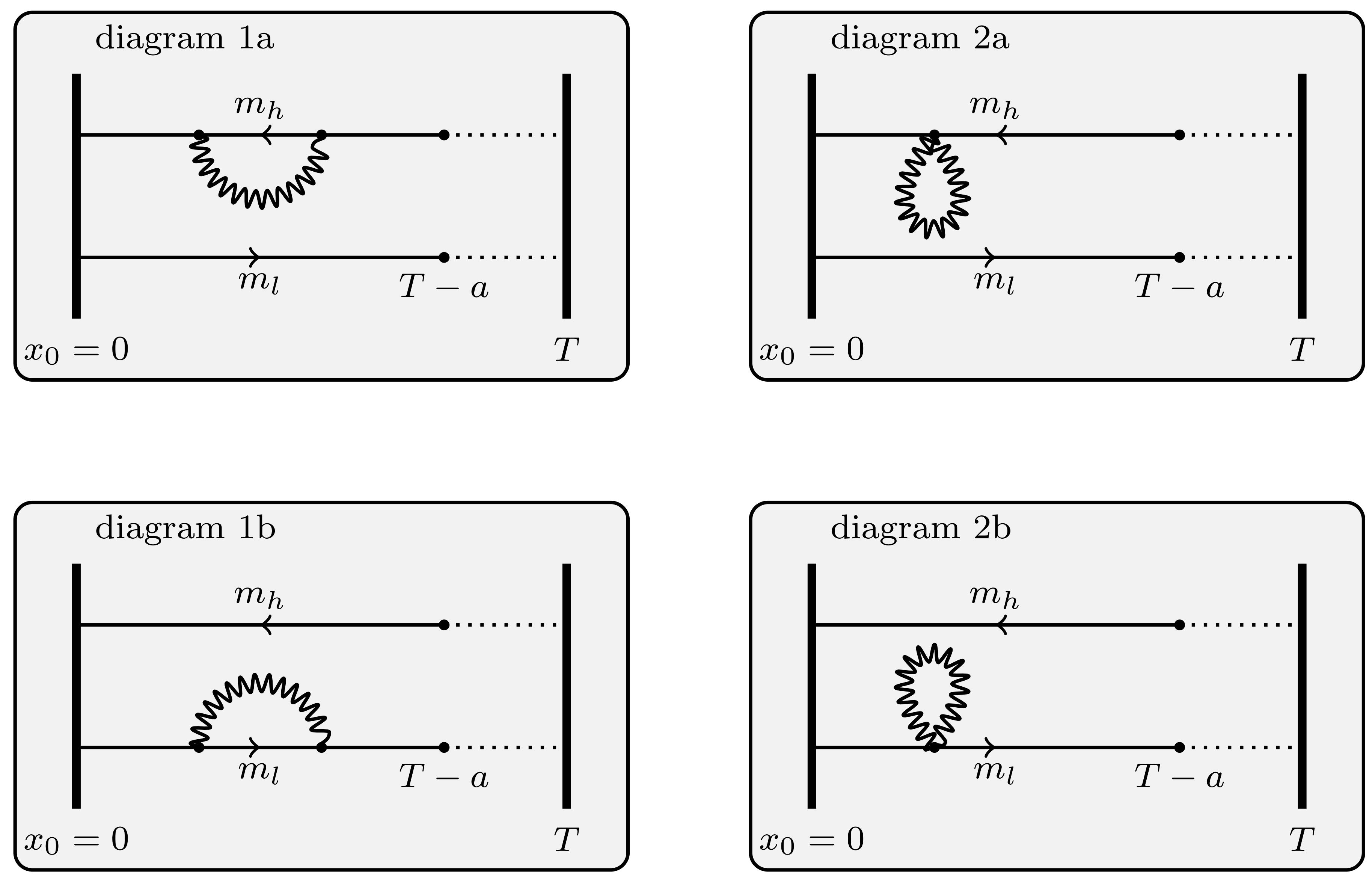
$$\mathcal{O}_{\rm spin}(x) = \overline{\psi}_{\rm h}(x)\,\sigma\cdot\mathbf{B}(x)\psi_{\rm h}(x),$$

$$\sigma_k = \frac{1}{2}\epsilon_{ijk}\sigma_{ij},$$

$$B_k(x) = \frac{i}{2}\epsilon_{ijk}\mathcal{F}_{ij}(x).$$

Round-off





Per-diagram comparison with data by Kurth and Sommer.

MC Cross Checks

We use pastor to calculate

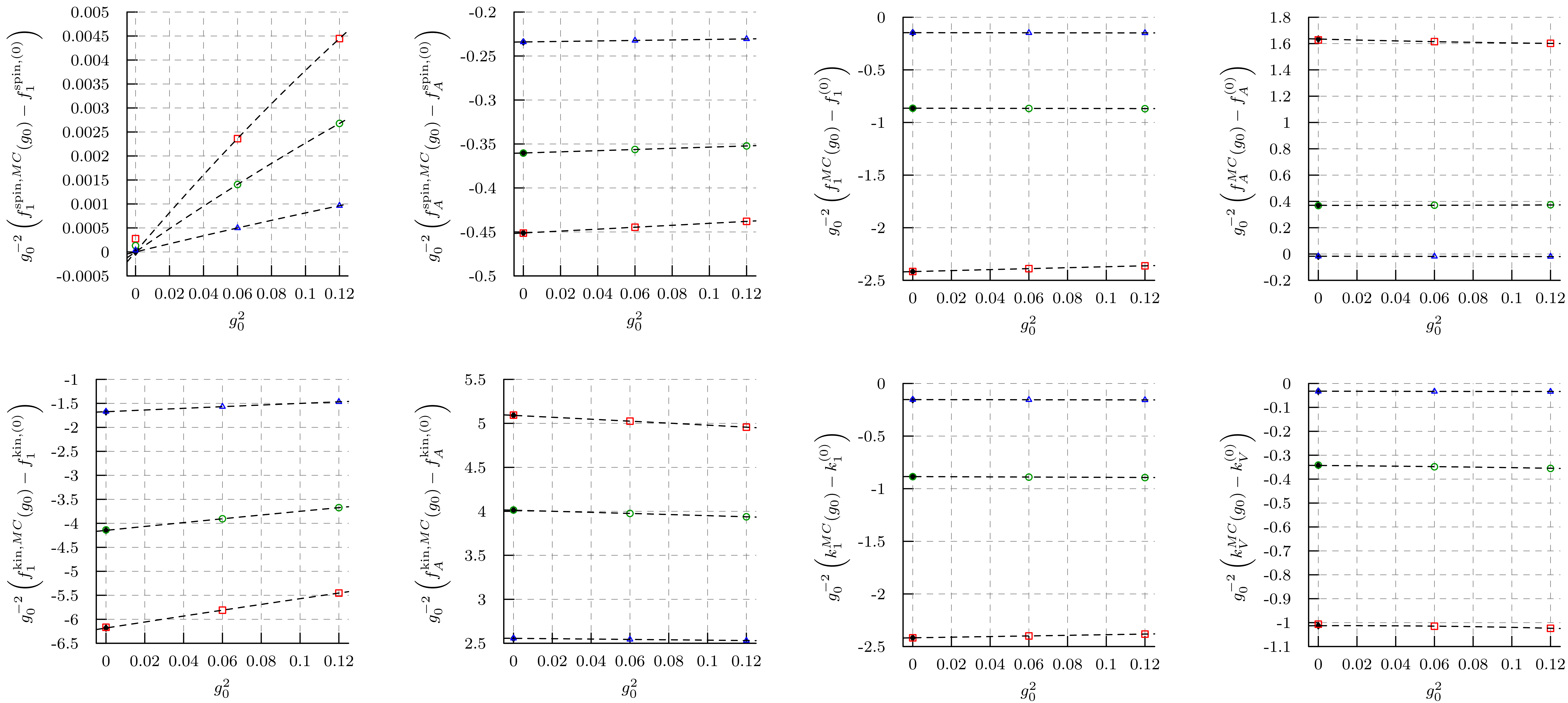
$$f(g_0) = f^{(0)} + g_0^2\, f^{(1)} + O(g_0^4)$$

We then extract an estimate for the one loop part from MC using

$$\tilde{f}^{(1)}(g_0) = g_0^{-2} \left(f^{MC}(g_0) - f^{(0)} \right)$$

and extrapolate linearly in g_0^2.

MC Cross Checks



Cross checks with MC data by Patrick Fritzsch.

Vertices - Details

The full result reads

$$\mathcal{U}^{(r)}(x,y) = \left(\frac{a}{L}\right)^{3r} \sum_{\mathbf{k}_1,a_1,\mu_1,t_1} \cdots \sum_{\mathbf{k}_r,a_r,\mu_r,t_r} q^{a_1}_{\mu_1}(\mathbf{k}_1;t_1)\ \ldots\ q^{a_r}_{\mu_r}(\mathbf{k}_r;t_r)$$
$$\times I_{a_r} \ldots I_{a_1} \sum_{0<u_1\leq\ldots\leq u_r\leq l}$$
$$\times \frac{r!}{\alpha_1!\ \ldots\ \alpha_l!} \prod_{j=1}^{r} s[u_j]\, \delta_{t[u_j],t_j}\ \delta_{\mu[u_j],\mu_j}\ e^{i\,\mathbf{k}_j \tilde{\mathbf{x}}[u_j]}.$$

This looks horrible, but can be constructed link by link defining an order-by-order multiplication

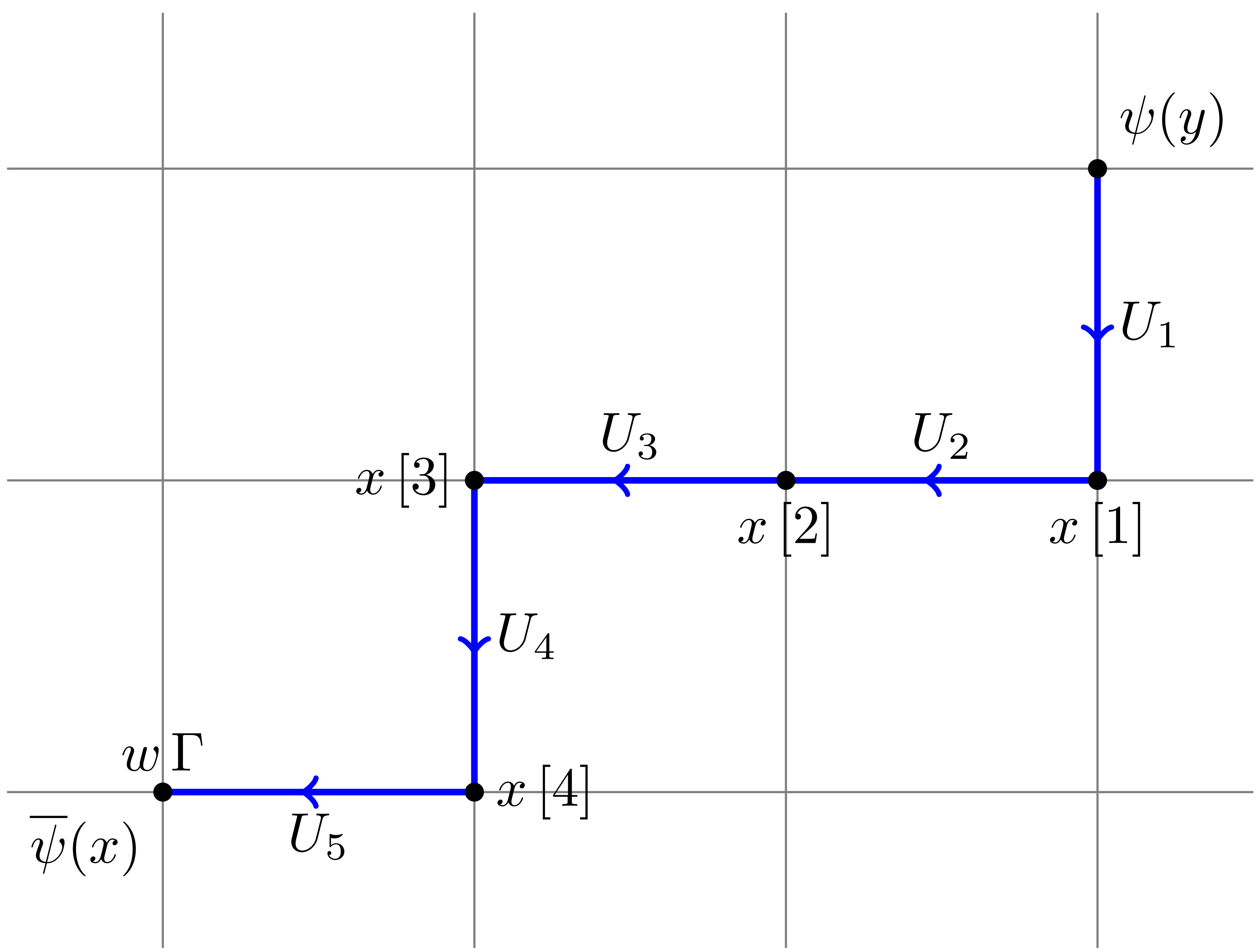
$$[U_\mu(x)\mathcal{U}(x,y)]^{(r)} = \sum_{s=0}^{r} U^{(s)}_\mu(x) \times \mathcal{U}^{(r-s)}(x,y).$$

The XML Input

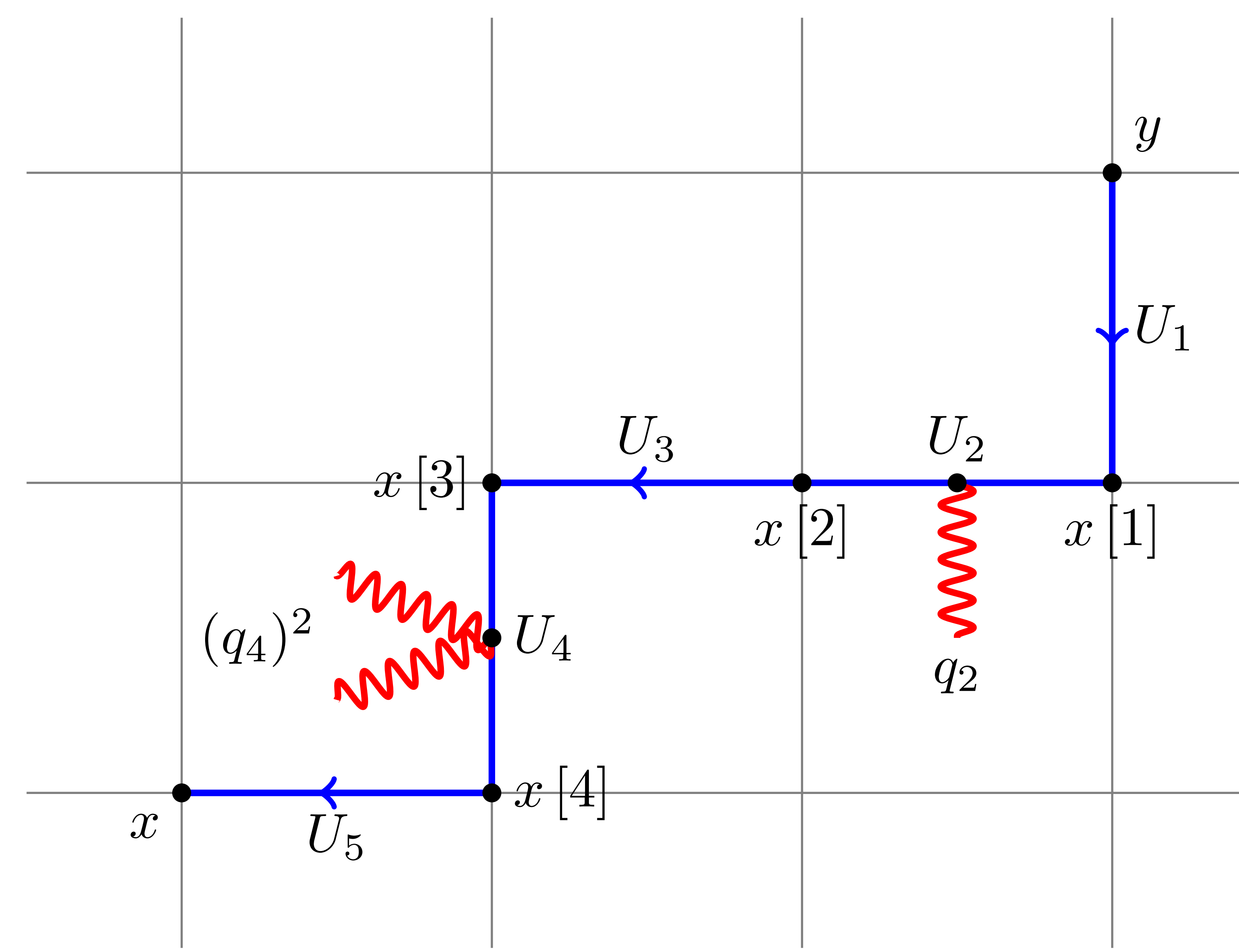
```xml
<boundary>
  <where>0</where> <!--x_0 = 0-->
  <spin>dirac</spin>
  <spins>15 -14</spins>
  <!-- 2 * P_+ * gamma_5 * P_- = -->
  <!-- 2 * gamma_5 * P_- = gamma_5 - gamma_5 * gamma_0 -->
</boundary>
<propagator>
  <thetax>theta</thetax> <!-- user parameter: theta-->
  <thetay>theta</thetay>
  <thetaz>theta</thetaz>
  <spin>dirac</spin>
  <action>HQET_stat</action>
  <!--from and to are optional tags, helping pastor to
      generate more efficient code -->
  <from>1</from>
  <to>x0</to>
</propagator>
```

Construction of a Vertex in Pictures

A parallel transporter like this:



Will yield $O\left(g_0^3\right)$ terms like this one:



Parse (and Compile)

GNU autotools make your life easy!

```
hal9000 | example_project $ ~/pastor-build/codegen/parse.py xml/phi_v0.xml

[...]

hal9000 | example_project $ cd source
hal9000 | source $ ./configure

[...]

hal9000 | source $ make
```

Run the Programs

f1_small_L.get file contents:

```
# Base path for the executables
BasePath /Users/dirk/tmp/pastor_build/codegen/example_project/source/
# Path for output and log files
WorkDir /Users/dirk/tmp/pastor_build/codegen/example_project/run/
# Bool (yes|no) if the propagators should be written
# to hard disk and their location
Propagators no -
# subdirectories and names for the observables
SubDir f1/.    f1_loop
SubDir f1/tree f1_tree
SubDir f1/db   f1_db
SubDir f1/dm   f1_dm
# Parameters can be given in various ways ...
# 4 to 8 in steps of 2
Parameter L 4:8:2
# formulae
Parameter T = L
Parameter x0 = T/2
# arrays
Parameter theta [0.0, 0.5, 1.0]
Parameter z [0, 1]
```

```
hal9000 | example_project $ ~/pastor-build/codegen/run.py xml/f1_small_L.get
```