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

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Outline

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

We want to evaluate expressions like this one:

\[ \sum_{p, y_0, z_0} \text{tr} \left\{ \begin{array}{c} \text{Diagram} \\ \tau = 0 \\ \tau = T \end{array} \right\} \]

With *automation* I mean automatic generation of Feynman diagrams *and* Feynman rules!
The Schrödinger Functional

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

\[ \bar{\zeta}(x) = \sum_y \psi(y)K(y, x), \quad \bar{\zeta}'(x) = \sum_y \psi(y)K'(y, x), \]

\[ P_+\psi(x)|_{x_0=0} = \bar{\psi}(x)P_-|_{x_0=0} = 0 \]

\[ P_-\psi(x)|_{x_0=T} = \bar{\psi}(x)P_+|_{x_0=T} = 0, \]

\[ P_\pm = 1/2(1 \pm \gamma_0) \]

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

This induces a background field,

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

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

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

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

Split up gauge and fermion averages, \( \langle O \rangle = \langle [O]_F \rangle_G \).

First perform fermion Wick contractions,

\[
\langle O \rangle = \langle \bar{\psi}_1(x) \gamma_5 \psi_2(x) \bar{\zeta}_2(y) \gamma_5 \zeta_1(z) \rangle_G
\]

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

Then the gauge average,

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

\[
Z_F[U] = \int D[\bar{\psi}, \psi] e^{-S_F[\bar{\psi}, \psi, U]}.
\]
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

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

For example

$$[\psi(x) \bar{\psi}(y)]_F = S(x, y),$$

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

M. Lüscher, P. Weisz, 1996.
ALPT - The Comic

Your favorite observable

Expand in powers of $g_0$

Fermion Wick contractions

Gluon Wick contractions

(plus many more!)
Perturbative Expansion

Now, expand

\[ S(x, y) = S^{(0)}(x, y) + g_0 S^{(1)}(x, y) + \ldots \]

\[ K(x, y) = K^{(0)}(x, y) + g_0 K^{(1)}(x, y) + \ldots \]

and perform the gluon Wick contractions.

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

\[
\left( D^{(0)} + m + g_0 D^{(1)} + \ldots \right) \left( S^{(0)}(x, y) + g_0 S^{(1)}(x, y) + \ldots \right) = \delta_{xy}
\]

order by order.

M. Lüscher, P. Weisz, 1996.
Fermion Actions

We assume that the fermion action looks like this

\[ S_F = \sum_i c_i \bar{\psi}(x_i) \Gamma_i U_i(x_i, y_i) \psi(y_i), \]

\[ U(x, y) = U_l U_{l-1} \ldots U_1, \]

\[ U_i = U_{s[i]\mu[i]}(x[i]), \quad U_{-\mu}(x) = U_{\mu}^\dagger(x - \hat{\mu}), \]

\[ s[i] \hat{\mu}[i] = x[i-1] - x[i], \quad x[0] = y. \]

For a given parallel transporter \( U(x, y) \)

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

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

General strategy:

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

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

\[
f(I) = \sum_{n=0}^{\infty} \frac{a_n + b_n \log I}{I^n} \quad I = \frac{L}{a}
\]

M. Lüscher, P. Weisz, 1996.

We extract the coefficients using successive fits.


Round-off errors can be estimated using long double precision.
Using pastor as an Aid for the Matching of HQET and QCD
Flavor Currents

\[
\left(V_{R}^{HQET}\right)_{0}(x) = Z_{V}^{HQET} \left[ V_{0}^{stat} + \sum_{i=1}^{2} c_{V}^{(i)} V_{0}^{(i)}(x) \right], \quad \left(V_{R}^{HQET}\right)_{k}(x) = Z_{V}^{HQET} \left[ V_{k}^{stat} + \sum_{i=3}^{6} c_{V}^{(i)} V_{k}^{(i)}(x) \right],
\]

\[
V_{0}^{stat}(x) = \overline{\psi}_{1}(x) \gamma_{0} \psi_{h}(x),
\]

\[
V_{0}^{(1)}(x) = \overline{\psi}_{1}(x) \frac{1}{2} \gamma_{i} \left( \nabla_{i}^{S} - \nabla_{i}^{S} \right) \psi_{h}(x),
\]

\[
V_{0}^{(2)}(x) = \overline{\psi}_{1}(x) \frac{1}{2} \gamma_{i} \left( \nabla_{i}^{S} + \nabla_{i}^{S} \right) \psi_{h}(x)
\]

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

\[
Z_{A}^{HQET}, Z_{A}^{HQET}, c_{A}^{(i)}
\]

In total 16 matching coefficients for the currents (plus 3 in the action)!
**Good Matching Conditions**

With correctly matched parameters, we expect

\[
X^{QCD}(m_h) = X^{\text{stat}} + O(1/m_h),
\]

\[
X^{QCD}(m_h) = X^{\text{stat}} + c_X X^{1/m_h} + \omega_{\text{kin}} X^{\text{kin}} + \omega_{\text{spin}} X^{\text{spin}} + O(1/m_h^2).
\]

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

\[ f_1^{V_0}(x_0; \theta, z = L m_3) = -\frac{1}{2} \sum_x \langle \bar{\zeta}_1 \gamma_5 \zeta_3 V_0(x) \bar{\zeta}_2 \gamma_5 \zeta'_1 \rangle, \]

\[ V_\mu(x) = \bar{\psi}_3(x) \gamma_\mu \psi_2(x), \quad \zeta_i = L^{-3/2} \sum_x \zeta_i(x) \]

which looks like this:

![Diagram showing the matching of the vector current with the given conditions.]
We also need the boundary-to-boundary correlator

\[ f_1(\theta, z) = -\left\langle \bar{\zeta}_2 \gamma_5 \zeta'_3 \bar{\zeta}_3 \gamma_5 \zeta_2 \right\rangle \]


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

\[ X_V(\mu) = Z_{A,\text{lat}}^{\text{stat}}(\mu) Z_{V/A}^{\text{stat}} X_V^{\text{bare}}, \quad X_V^{\text{bare}} = \frac{\left(f_{V_0}^{\text{stat}}\right)^{\text{stat}}(T/2; \theta)}{\sqrt{f_1^{\text{stat}}(\theta)f_1(\theta, 0)}}, \]

\[ Z_{A,\text{lat}}^{\text{stat}}(\mu) = 1 - \gamma_0 \log(a\mu) g_0^2 + O(g_0^4). \]

One may then expect that up to one loop

\[ \Phi^{V_0}(z) = (1 + B_A^{\text{stat}}g_0^2)X_V(z/L) + O(1/z). \]

Tree Level

\[ \phi_{V_0,0}(0) \]

\[ \frac{1}{z} \]

\( \theta = 0.0 \)
\( \theta = 0.5 \)
\( \theta = 1.0 \)
One Loop - Theory

We define the quantity

\[ Y_{V}^{(1)} = \Phi^{V_{0},(1)}(z) - \left[ B_{V}^{\text{stat}} - \gamma_{0} \log(z) + \left( Z_{V/A}^{\text{stat}} \right)^{(1)} \right] X_{V}^{(0)} , \]

and may expect that

\[ Y_{V}^{(1)}(z) \xrightarrow{1/z \to 0} X_{V,\text{lat}}^{(1)} = X_{V}^{\text{bare},(1)} - \gamma_{0} \log(a/L) X_{V}^{\text{bare},(0)} . \]

(“lat” = lattice minimal subtraction)
One Loop - Results

The fit functions have the form

\[ Y_V^{(1)}(z) = X_{V,\text{lat}}^{(1)} + c_1/z + c_2/z^2. \]

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

Diagram count

<table>
<thead>
<tr>
<th></th>
<th>QCD</th>
<th>static</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_1^{V0}$</td>
<td>30</td>
<td>29</td>
</tr>
<tr>
<td>$f_1$</td>
<td>22</td>
<td>21</td>
</tr>
</tbody>
</table>

Three values for $\theta$

$L/a = 4,\ldots,40$

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

\[ \mathcal{O}_{\text{kin}}(x) = \bar{\psi}_h(x) \nabla^* \nabla_k \psi_h(x), \]
\[ \mathcal{O}_{\text{spin}}(x) = \bar{\psi}_h(x) \sigma \cdot \mathbf{B}(x) \psi_h(x), \]
\[ \sigma_k = \frac{1}{2} \epsilon_{ijk} \sigma_{ij}, \]
\[ B_k(x) = \frac{i}{2} \epsilon_{ijk} \mathcal{F}_{ij}(x). \]
4. Cross Checks

Since the diagrams of type "2" have only one vertex, the number of additions decreases significantly. The rising of the relative errors in the figure is compatible with this behavior as suggested by the fit functions.

The numerical values for these diagrams were provided by the authors of [19] and we refrain from performing a fit in this case.

Relative round-off errors were performed up to sufficiently large lattice sizes \((L/a)\). We estimated the round-off error and fitted using the function \(\ln(L/a) = A_0 + A_1 \ln(L/a) + A_2 \ln(L/a)^2 \) at order \(\theta = 0\), \(A_1 = 0\) requires \(\delta_{\text{stat}}\) as introduced in [20].

As a first check, we compared data calculated with data types and comparing the results instead of using the same data type. For a representative set of observables, calculations in both levels of precision were performed up to 1e-15 and we refrain from performing a fit in this case.

Errors are smaller. The spread of the errors is rather large.

The numerical results of the two calculations for \(L/a = 8\) and \(L/a = 20\) are included. The agreement within round-off error for diagrams contributing to spin \(1/2\) is such that the round-off error and the round-off reference parameter \(O\) were assumed to represent the round-off error and fitted using the function \(\delta = B_0 + B_1 \ln(L/a) + B_2 \ln(L/a)^2\).

The diagram of type "2" has two vertices and we refrain from performing a fit in this case.

We may now write \(A_Z \mathcal{H}_{\text{QCD}}(z) = \mathcal{H}_{\text{QCD}}(z)\), \(\mathcal{H}_{\text{QCD}}(z)\), \(\mathcal{H}_{\text{QCD}}(z)\), and \(\mathcal{H}_{\text{QCD}}(z)\) at order \(\theta = 0\). The magnitude of the relative di

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 \( g_0^2 \).
Cross checks with MC data by Patrick Fritzsch.
The full result reads

\[ \mathcal{U}^{(r)}(x, y) = \left( \frac{a}{L} \right)^{3r} \sum_{k_1, a_1, \mu_1, t_1} \cdots \sum_{k_r, a_r, \mu_r, t_r} q^{a_1}_{\mu_1}(k_1, t_1) \cdots q^{a_r}_{\mu_r}(k_r, t_r) \]

\[ \times I_{a_r} \cdots I_{a_1} \sum_{0 < u_1 \leq \ldots \leq u_r \leq l} \]

\[ \times \frac{r!}{\alpha_1! \cdots \alpha_l!} \prod_{j=1}^{r} s[u_j] \delta_{t[u_j], t_j} \delta_{\mu[u_j], \mu_j} e^{i k_j \tilde{x}[u_j]} \].

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

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

```bash
# 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