Hopping Parameter Expansion for Heavy-Light Systems

*UKQCD Collaboration*

D.S. Henty and R.D. Kenway
Department of Physics, The University of Edinburgh, Edinburgh EH9 3JZ, Scotland

**Abstract**

We present a technique which permits the calculation of two-point functions of operators containing one heavy quark and an arbitrary number of light quarks as analytic functions of the heavy-quark mass. It is based on the standard Jacobi linear solver used for the calculation of quark propagators. Results for the heavy-light pseudoscalar and vector meson masses are obtained on $16^3 \times 48$ lattices at $\beta = 6.2$ using the Wilson fermion action, and agree with published data. The incorporation of smeared operators and $O(a)$-improved actions presents no problems.
Introduction There is much interest at present in studying systems involving both heavy and light quarks on the lattice. The reasons for this are twofold. Firstly, the values of quantities such as the decay constants of the $D$ and $B$ mesons and the form of the Isgur-Wise function \cite{1} are currently of great interest to both the experimental and theoretical communities. These are, in principle, calculable on the lattice. Secondly, it is expected that discretisation errors are relatively large for states containing heavy quarks and such systems provide an arena in which to look for gains from the use of improved actions \cite{2}.

Although nature has so far only revealed two heavy quarks, charm and bottom, with masses of approximately 1.5 and 5 GeV respectively, it is not always sufficient to perform lattice simulations solely at these two points. Regarding the evaluation of the Isgur-Wise function $\xi(v,v')$, it is essential to know when (and if) the heavy-quark effective theory is valid. Once this has been determined, it is necessary to perform measurements at many different heavy-quark velocities to map out the form of $\xi(v,v')$. Since the lattice quantises the allowed values of momenta, this can only be done in a continuous fashion by varying the quark mass. In order to study lattice artifacts we need to have results at many heavy-quark masses to discover when and how the discretisation errors manifest themselves and to decide when to trust the lattice results.

In this letter, we use the standard Wilson fermion action

$$S_W^F = \sum_x \left\{ \bar{q}(x)q(x) - \kappa \sum_\mu \left[ \bar{q}(x)(1 - \gamma_\mu)U_\mu(x)q(x + \hat{\mu}) + \bar{q}(x + \hat{\mu})(1 + \gamma_\mu)U_\mu^\dagger(x)q(x) \right] \right\} = \bar{q}(1 - \kappa D)q$$

where $\kappa$, the quark hopping parameter, is inversely related to the bare mass. We develop a method which allows the hadron correlators to be evaluated as convergent power series in the heavy-quark hopping parameter. In what follows we denote generic quarks and their hopping parameters by $q$, $\bar{q}$ and $\kappa$, and use $h$, $\bar{h}$ and $\kappa_h$ for heavy quarks.

Jacobi Algorithm To evaluate any lattice quark propagator $G$ we need to solve the linear equation

$$(1 - \kappa D)G = \eta$$

for $G$ with some given source $\eta$. The Jacobi algorithm comes from the naïve Taylor expansion of the inverse of the fermion matrix, \textit{i.e.}

$$G = \eta + \sum_{n=1}^{\infty} \kappa^n D^n \eta.$$ 

In practice, it is implemented by the recursion relation

$$G_0 = \eta$$

$$G_{n+1} = \eta + \kappa D G_n$$

(4)
where we terminate the series at some finite \( n_{\text{max}} \). The minimum value of \( n_{\text{max}} \) needed to achieve some desired accuracy can be chosen, for example, by monitoring the norm of the residue vector

\[
 r_n = \eta - (1 - \kappa \mathcal{P}) G_n. \tag{5}
\]

The algorithm is convergent for sufficiently small \( \kappa \), and for the heavy-quark masses of interest there is no problem with convergence. For our purposes it is sufficient to notice that at iteration \( n \), \( G_n \) is updated by a term of order \( \kappa^n \).

Dividing the lattice into even and odd sites and using the fact that \( \mathcal{P} \) only connects even sites to odd sites it is apparent that the solution \( G \) of equation (2) satisfies

\[
 G_{\text{odd}} = \eta_{\text{odd}} + \kappa \mathcal{P} G_{\text{even}} \tag{6}
\]

We need only compute the solution on even sites which satisfies

\[
 (1 - \kappa^2 \mathcal{P}^2) G_{\text{even}} = \eta_{\text{even}} + \kappa \mathcal{P} \eta_{\text{odd}} \tag{7}
\]

Equations (6) and (7) comprise the red-black preconditioning of equation (4) and for the Jacobi algorithm reduce the computational load by a factor of two.

**Hopping Parameter Expansion** For simplicity, consider a mesonic operator \( \mathcal{O} \Gamma = \bar{h} \Gamma q \). The quantity of interest is the timesliced correlator \( C_{\Gamma}(t) \) defined by

\[
 C_{\Gamma}(t) = \sum_{\vec{x}} \langle \mathcal{O}_{\Gamma}(\vec{x}, t) \mathcal{O}_{\Gamma}^\dagger(0, 0) \rangle \\
 = \sum_{\vec{x}} \langle \text{Tr} \left\{ \gamma_5 \Gamma G_q(\vec{x}, t) \bar{\Gamma} \gamma_5 \Gamma h_{\vec{x}}(\vec{x}, t) \right\} \rangle \tag{8}
\]

where \( \bar{\Gamma} = \gamma_0 \Gamma^\dagger \gamma_0 \). We assume that the computationally intensive part of this calculation (the evaluation of the light quark propagator \( G_q \)) has been performed. Using the Jacobi algorithm, the standard approach would be to solve the red-black preconditioned equation (7) for some particular value of \( \kappa_h \) and compute \( G_h \). \( C_{\Gamma}(t) \) would then be evaluated and the whole procedure repeated for each different value of \( \kappa_h \).

We introduce the hopping parameter expansion [3] by inserting the Taylor series expansion for \( G_h \) directly into equation (8) to obtain \( C_{\Gamma}(t) \) as a power series in \( \kappa_h \):

\[
 C_{\Gamma}(t) \approx \sum_{n=0}^{n_{\text{max}}} c_{\Gamma}^{(n)}(t) \kappa_h^n \tag{9}
\]

where

\[
 c_{\Gamma}^{(n)}(t) = \sum_{\vec{x}} \langle \text{Tr} \left\{ \gamma_5 \Gamma G_q(\vec{x}, t) \bar{\Gamma} \gamma_5 \mathcal{P}^n \eta^\dagger (\vec{x}, t) \right\} \rangle \tag{10}
\]

and \( \mathcal{P}^0 \eta = \eta \).
The computational overhead is the calculation of the desired traces at every order of the expansion rather than only once for the sum of the series. The gain is that the light quark propagator only has to be read in to memory once, which may be significant on certain machines for large lattices, and results are obtained for a continuous range of \( \kappa_h \).

It is obvious that the static approximation (the limit of infinite quark mass / zero \( \kappa_h \)) is a simple by-product of this more general finite mass expansion. The relationship is

\[
C_{\Gamma}^{\text{static}}(t) = c_{\Gamma}^{(t)}(t). \tag{11}
\]

The numerical problem with equation (9) as it stands is that the coefficients \( c_{\Gamma}^{(n)}(t) \) diverge as \( n \) becomes large and eventually cause an overflow on the computer. We can predict the growth of \( c_{\Gamma}^{(n)}(t) \) by the following simple argument.

Consider the pseudoscalar channel \( (\Gamma = \gamma_5) \). At some critical value of the hopping parameter \( \kappa = \kappa_c \), the pseudoscalar comprising two degenerate light quarks (the pion) becomes massless. In this case \( C_{\Gamma}(t) \) no longer decays exponentially and so we expect all orders of the hopping parameter expansion to contribute with roughly equal weight, \textit{i.e.}

\[
c_{\gamma_5}^{(n)}(t) \kappa_c^n \sim \text{constant}. \tag{12}
\]

Since the pseudoscalar is the lightest channel, \( c_{\gamma_5}^{(n)}(t) \) will have the worst divergences. If we can keep these under control, then all other channels will be numerically stable as well.

Thus, although in practice we deal with light quark propagators which correspond more to the strange quark mass than the chiral limit, if we rewrite equation (9) as

\[
C_{\Gamma}(t) \simeq \sum_{n=0}^{n_{\text{max}}} c_{\Gamma}^{(n)}(t) [\alpha \kappa_h]^n \tag{13}
\]

with \( \alpha \sim \kappa_c^{-1} \) then we expect the new expansion coefficients \( \bar{c}_{\Gamma}^{(n)}(t) \) to be roughly constant.

**Simulation Details** Numerical studies were performed on 10 lattices of size \( 16^3 \times 48 \), generated in the quenched approximation at \( \beta = 6.2 \). Since the major purpose of this letter is to demonstrate the validity of the technique and to reproduce known results, only two meson operators were calculated:

\[
\begin{align*}
\text{Pseudoscalar : } & \Gamma = \gamma_5 \\
\text{Vector : } & \Gamma = \sum_{i=1}^{3} \gamma_i
\end{align*}
\]

from which the masses and hyperfine splitting can be calculated and compared to reference [4]. The light-quark hopping parameter was chosen as \( \kappa = 0.1510 \), corresponding roughly to the strange quark mass [4], and these light propagators were calculated using an over-relaxed minimal residual algorithm. To span the range of heavy-quark masses in [4] (0.125 \leq
The hopping parameter expansion was computed to 200th order. This number was chosen by explicitly calculating quark propagators at \( \kappa_h = 0.145 \) using the Jacobi algorithm and requiring that the residue vector of equation (5) satisfy \(|r_{n_{\text{max}}}| < 10^{-7}\). The following test was performed on a single configuration. Firstly, the standard propagator code (used to evaluate the light propagator) was used to compute the heavy-quark propagators at \( \kappa_h = 0.145 \) and \( \kappa_h = 0.125 \), and the values of \( C_V(t) \) calculated directly. Secondly, the coefficients \( \bar{c}_{\Gamma}^{(n)}(t) \) were computed and the series summed off-line at the same two values of \( \kappa_h \). The results are illustrated in figure 1, where the solid line is the hopping parameter expansion summed to a given order and the dashed line is the value of \( C_V(t) \). The results of these two independent calculations agreed, and it was deduced that the hopping parameter expansion had converged (to the accuracy desired) within the required range. As expected, convergence is most rapid at small values of \( \kappa_h \) and \( t \). The other notable features are that the convergence of neither the vector nor the pseudoscalar meson correlators is monotonic, and that the full 200 orders are necessary at the lightest mass and furthest timeslice. For heavy quarks near the charm mass (\( \kappa_h \approx 0.135 \)) around 100 orders are sufficient.

The value of \( \alpha \) was varied, and the scaled coefficients \( \tilde{c}_{\Gamma}^{(n)}(t) \) found to be numerically stable for \( \alpha = 6.0 \). The bare coefficients \( c_{\gamma_5}^{(n)}(t) \) actually grow like \((6.3)^n\) which, since the critical
hopping parameter $\kappa_c \simeq 0.1533$, agrees with our prediction $c^{(n)}_\gamma(t) \sim (6.5)^n$.

For these initial studies, point sources at the origin (an even site) and point sinks were used for both the heavy and the light quarks. In this case, the hopping parameter expansion is an implementation of the red-black preconditioned Jacobi algorithm. Although our tests, performed on a single configuration, were sufficient to prove that the algorithm works we decided to use smeared operators during the full simulation in order to obtain better signals for the relevant particles. Point sources were still used for the heavy quarks so that the red-black factorisation could be exploited. The light-quark operators were smeared at the source and the sink using a gauge covariant smearing function with an RMS smearing radius of about four lattice spacings. The incorporation of non-local heavy-quark sources and sinks is discussed later.

**Results** Since in principle the simulation provides $C_\Gamma(t)$ as an analytic function of $\kappa_h$ there are several analysis methods available. Previously, when the expansion was truncated well before convergence, the behaviour of the Fourier transformed correlation functions was studied and the particle masses identified as poles in momentum space. Our approach is to sum the series at many values of $\kappa_h$ and fit the asymptotic exponential decay in time.

After the use of smeared operators, plateau regions in $C_\Gamma(t)$ were readily identified for the whole range of $\kappa_h$, although the limited statistics meant that the signal deteriorated rapidly especially at very large heavy-quark masses (here we approach the static quark limit where this effect is well known). An uncorrelated fit to the vector and pseudoscalar meson channels was done from time slices 5 to 10 and the corresponding masses extracted. To estimate the errors, the whole procedure was bootstrapped and the probability distributions of the masses and mass difference obtained. The quoted errors are 68% confidence level regions and are therefore not necessarily symmetric. Unfortunately, lack of statistics prevented a proper correlated fit.

The most interesting quantity is $m_V^2 - m_P^2$, which becomes constant in the heavy-quark effective theory with corrections of order $(m_V + m_P)^{-1}$. Experimentally, this quantity is remarkably constant all the way from the $\pi, \rho$ system through the $K$ and $D$ to the $B$, with a measured value of around 0.55 GeV$^2$. We plot this mass difference against $m_P^2$ in figure 2 together with the data from [4]. Our analysis was actually done at 17 evenly spaced values of $\kappa_h$, and we have drawn a continuous line representing the best fits and dashed lines representing the envelope of the error bars. It is clear that, within errors, there is no discrepancy between the two data sets. The results show the well-known feature that the hyperfine splitting for heavy-quark mesons is far too small for the Wilson action (at $\beta = 6.2, a^{-1} = 2.73$ GeV) and decreases with increasing heavy-quark mass, contrary to experiment. This is observed both in heavy-light and heavy-heavy systems.
Non-Local Operators and Improved Actions  It is not practical to smear the heavy-quark propagator at the sink since this would have to be done at each order of the hopping parameter expansion, taking a prohibitively long time for even the simplest of smearing techniques. If smearing is required at the sink, it should be performed on the light quark fields as this only needs to be done once. The only complication arises if smearing is required at the source because the only light-quark propagators available originate from point sources. In this case, it is necessary to smear the heavy quark at the source. There is no problem in doing this, the only disadvantage being that the red-black factorisation cannot be exploited.

It has been suggested that the unphysically small value obtained for the hyperfine splitting in heavy-quark systems is due to large order $a$ effects present in the Wilson action. Using an $O(a)$-improved fermion action would be expected to improve the situation, and this has been demonstrated for the “clover” action by studying the charmonium system \cite{7,6}. The important point is that $\kappa$ still only enters the fermion action as an overall prefactor so it is straightforward to use the hopping parameter expansion. The other element of the clover action is that the quark propagator needs to be rotated at source and sink to complete the $O(a)$ improvement \cite{2}, so there is no advantage to red-black factorisation.

Conclusions  We have shown that the hopping parameter expansion is a viable method for the study of heavy-light systems on the lattice. It provides results as an analytic function of the heavy-quark mass provided that this mass is larger than some lower bound. This lower bound can be reduced by going to higher orders of the expansion, but for studies at $\beta = 6.2$
on a $16^3 \times 48$ lattice only 200 orders are needed for $\kappa_h \leq 0.145$. This is lighter than charm for which $\kappa_h \simeq 0.135$ and where around 100 orders are sufficient. The hopping parameter expansion, when used with an $O(a)$-improved action, provides an attractive method for mapping out the behaviour of meson decay constants and the Isgur-Wise function continuously at and above the charm quark mass.

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