Detector resolution effects on hadronic mass moments in $B \to X\ell\nu$

Christian W. Bauer$^{1,*}$ and Benjamin Grinstein$^{1,†}$

$^1$Department of Physics, University of California at San Diego, La Jolla, CA 92093

We show how to relate moments of the reconstructed hadronic invariant mass distribution to the moments of the physical spectrum in a model independent way. The only information needed on detector resolution functions are their first few moments. Theoretical predictions for the first three moments as functions of non-perturbative parameters are given for various lepton energy cuts.

Differential distribution for inclusive decay rates of heavy mesons can be calculated using the operator product expansion (OPE) [1]. The resulting decay distributions are singular and can only be compared with experimentally measured distributions after smearing them over a sufficiently large interval. For example, calculating the hadronic invariant mass distribution for the semileptonic decay $B \to X_c\ell\bar{\nu}$ using the OPE, one finds to leading order in $\Lambda_{\text{QCD}}/m_b$ [2]

$$\frac{d\Gamma}{ds} = \Gamma \delta(s - m_D^2) + O\left(\frac{\Lambda_{\text{QCD}}}{m_b}\right),$$

where $s = m_X^2$ is the square of the hadronic invariant mass, $m_D = \frac{1}{2}(m_D + 3m_{D^*})$ is the spin averaged $D$-$D^*$ mass, and $\Gamma$ denotes the total semileptonic width. Non-perturbative corrections to this differential rate yield even more singular terms. To compare this distribution with the smooth spectrum measured experimentally, one has to find observables which sufficiently smear the differential spectrum. The simplest such observables are moments of this spectrum, defined as

$$M_n = \frac{\int ds \, s^n \frac{d\Gamma}{ds}}{\int ds \, \frac{d\Gamma}{ds}}.$$  

(2)

From Eq. (1) on obtains trivially

$$M_n = m_D^{2n} \left[ 1 + O\left(\frac{\Lambda_{\text{QCD}}}{m_b}\right) \right].$$

(3)

The corrections to the first two moments have been calculated to order $1/m_b^3$ and $\alpha_s^2\beta_0$ [2–4]. By measuring deviations from the above relation, one can therefore obtain information about the size of the non-perturbative matrix elements. In turn, information on these non-perturbative parameters can be used in precise determination of CKM elements $|V_{cb}|$ and $|V_{ub}|$.

The first two moments were first measured by the CLEO collaboration with a lower cut on the lepton energy, to suppress the background in which the lepton originates from a semileptonic decay of the $D$ meson [5]. More recently, the DELPHI collaboration presented measurements of these moments without a cut on the lepton energy [6], while the BaBar collaboration measured the first moment as a function of the lepton energy cut [7]. This dependence on the lepton energy cut can be compared with predictions from theory, allowing for a more detailed test of the operator product expansion.

In general, the reconstructed hadronic invariant mass spectrum $d\Gamma/ds_R$ is a convolution of the true spectrum $d\Gamma/dsT$ and a detector resolution function $P(s_R - s_T, s_T)$, which describes the probability of measuring the reconstructed invariant mass $s_R$, given the true mass $s_T$

$$\frac{d\Gamma}{ds_R} = \int ds_T \left[ P_D(s_R - s_T, s_T, E_{\text{cut}}) \frac{d\Gamma_D}{ds_T} |_{E_{\text{cut}}} ight. + P_{D^*}(s_R - s_T, s_T, E_{\text{cut}}) \frac{d\Gamma_{D^*}}{ds_T} |_{E_{\text{cut}}} + P_X(s_R - s_T, s_T, E_{\text{cut}}) \frac{d\Gamma_X}{ds_T} |_{E_{\text{cut}}} \right],$$

(4)

where $X$ denotes any charmed final state not equal to a single $D$ or $D^*$. In (4) we have allowed for different resolution functions for $D$, $D^*$ and $X$ final states as is expected experimentally. Each term in this expression depends explicitly on the value of the lepton energy cut $E_{\text{cut}}$. In the remainder of this paper, this dependence will be suppressed, however all equations should be understood as having this dependence.

From the result of [2–4] for the first two moments of the differential decay spectrum

$$\frac{d\Gamma}{ds} = \frac{d\Gamma_D}{ds} + \frac{d\Gamma_{D^*}}{ds} + \frac{d\Gamma_X}{ds}$$

(5)

we can then obtain the spectra needed in (4) using

$$\frac{d\Gamma_D}{ds} = \Gamma_D \delta(s - m_D^2)$$

(6)

$$\frac{d\Gamma_{D^*}}{ds} = \Gamma_{D^*} \delta(s - m_{D^*}^2)$$

(7)

$$\frac{d\Gamma_X}{ds} = \frac{d\Gamma}{ds} - \frac{d\Gamma_D}{ds} - \frac{d\Gamma_{D^*}}{ds}$$

(8)

where $\Gamma_D$, $\Gamma_{D^*}(E_{\text{cut}})$ are the decay rates for $B \to D(D^*)\ell\bar{\nu}$ in the presence of a lepton energy cut. Note that only for $E_{\text{cut}} = 0$ can the values of $\Gamma_D$ be obtained from the measured branching fractions.

As explained above, the theoretical expression for the differential decay rate is given in terms of a singular expansion. Thus, this spectrum can only be compared with

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*Electronic address: bauer@physics.ucsd.edu
†Electronic address: bgrinstein@ucsd.edu
the experimentally measured spectrum after smearing it with some appropriate weight function. One can show that this weight function has to be a smooth function with width of order $\sqrt{m_b \Lambda_{\text{QCD}}}$. While the detector resolution function does provide a smeared spectrum of the theoretical spectrum, its width is only several hundred MeV [7]. Thus, additional smearing is required to compare the calculated spectrum with the measured spectrum. The simplest observables to compare are moments of the reconstructed hadron invariant mass spectrum.

These moments can easily be obtained from the general expression given in Eq. (4)

$$
\langle (s_R - \overline{m}^2_D)^N \rangle = \frac{1}{\Gamma} \int ds_R (s_R - \overline{m}^2_D)^N \frac{d\Gamma}{ds_R}
$$

$$
= \frac{1}{\Gamma} \int ds_T \left[ P_D^n(s_T) \frac{d\Gamma_D}{ds_T} + P_D^n(st_T) \frac{d\Gamma_D}{ds_T} 
+ P_X^n(st_T) \frac{d\Gamma_X}{ds_T} \right]. \tag{9}
$$

Here we have defined

$$
P^n(s_T) = \int ds_R (s_R - \overline{m}^2_D)^N P(s_R - s_T, s_T), \tag{10}
$$

where $P$ stands for any of the three resolution functions. Thus, moments of the reconstructed spectrum are given by the true spectrum, weighted with a function which is determined by the detector response.

The result in Eq. (6) can be further simplified by expanding the functions $P^n(s_T)$ in a Taylor series:

$$
P^n(s_T) = \sum_n (s_T - \overline{m}^2_D)^n P^n
$$

The coefficients $P^n$ depend on the precise form of the detector resolution function, but we can obtain some estimates using the expected form of the detector resolution function. We expect that for a given value of $s_T$ the function $P(\omega, s_T)$ is peaked around $\omega = 0$ with some width $\sigma$ that may depend weakly on $s_T$. The resolution functions used by the Babar collaboration [7] have width of order $\sigma \sim 1 \text{ GeV}^2$, while for a measurement using fully reconstructed $B$ events we expect $\sigma \sim (700 \text{ MeV})^2$. We furthermore assume that for a variation in the resolution function are slow compared to the width of the resolution function. If the width $\sigma$ varies by a small fraction $\epsilon$ over the range of the hadronic mass,

$$
\frac{d^n \sigma}{d s_T^n} \sim \left( \frac{s_T^\text{max} - s_T^\text{min}}{T} \right)^n \sim \epsilon \frac{\sigma}{m_B^n}
$$

then the coefficients $P^n$ are suppressed by $\epsilon$ for $n > N$:

$$
P^n \sim \left\{ \begin{array}{ll}
\frac{\sigma^{N-n}}{m_B^{n-n}} & \text{for } n \leq N \\
\epsilon \frac{\sigma}{m_B^n} & \text{for } n > N \end{array} \right. \tag{13}
$$

We can now see how the expected form of the resolution function results in a simple organization of the expansion (11). Using the estimates (13) and $\langle (s_T - \overline{m}^2_D)^n \rangle \sim \lambda_{\text{QCD}}^2$ we estimate the different terms in Eq. (11) as follows:

$$
\langle (s_R - \overline{m}^2_D)^N \rangle \sim \sum_{n=0}^N \sigma^{N-n} \lambda_{\text{QCD}}^{2n} + \sum_{n>N} \epsilon \frac{\sigma}{m_B^n} \lambda_{\text{QCD}}^{2n} \tag{14}
$$

Thus, if the resolution functions behave as expected, the terms with $n \geq N + 1$ in the relation (14) giving the measured moments in terms of the theory moments are suppressed by $\epsilon \frac{\sigma}{m_B^n} \lambda_{\text{QCD}}^{2n}$. Note also that since present experiments have $\sigma$ substantially larger than $\lambda_{\text{QCD}}$, the contributions of low $n$ theory moments to the measured $N$-th moment are amplified by powers of $\sigma/\lambda_{\text{QCD}}^2$. Neglecting the suppressed terms ($n \geq N + 1$) we thus obtain

$$
\langle (s_R - \overline{m}^2_D)^N \rangle = \sum_{n=0}^N \left[ \Gamma_D \left( \frac{P_D^n(s_T, s_T)}{m_B^n} - \overline{m}^2_D \right)^n 
+ \Gamma_D \left( \frac{P_D^n(s_T, s_T)}{m_B^n} - \overline{m}^2_D \right)^n 
+ \frac{P_X^n((s_T - \overline{m}^2_D)^n)}{m_B^n} \right]. \tag{15}
$$

This is the main result of this paper and shows how moments of the reconstructed hadronic invariant mass are related to the moments of the true mass distribution. The only ingredient in this relation are the first few moments of the detector resolution functions.

As an example of these simplifications we consider a simple model for the detector resolution function

$$
\bar{P}(\omega, s_T) = \frac{1}{\sqrt{2\pi}} \frac{1}{\Delta(s_T)} \exp \left[ -\frac{\omega^2}{2\Delta(s_T)^2} \right] \tag{16}
$$

Here, the width of the Gaussian distribution depends on the value of $s_T$, however the variation is slow compared to the width of the Gaussian itself

$$
\frac{d^n \Delta(s_T)}{d s_T^n} \sim \epsilon \frac{\Delta(\overline{m}_D^2)}{m_B^n} \tag{17}
$$

For this model the Taylor expansions of the first few functions $P^n$, Eq. (11), are

$$
P^0(s_T) = 1
$$

$$
P^1(s_T) = (s_T - \overline{m}^2_D)
$$

$$
P^2(s_T) = (s_T - \overline{m}^2_D)^2 + \Delta(\overline{m}_D^2)
$$

$$
= \Delta(\overline{m}_D^2)^2 + 2 \Delta(\overline{m}_D^2) \Delta'(\overline{m}_D^2)(s_T - \overline{m}_D^2)
+ \left[ 1 + (\Delta'(\overline{m}_D^2))^2 + \Delta(\overline{m}_D^2) \Delta''(\overline{m}_D^2) \right] (s_T - \overline{m}_D^2)^2
+ \left[ \Delta'(\overline{m}_D^2) \Delta''(\overline{m}_D^2) + \frac{\Delta(\overline{m}_D^2) \Delta'''(\overline{m}_D^2)}{3} \right] (s_T - \overline{m}_D^2)^3
+ O((s_T - \overline{m}^2_D)^4) \tag{18}
$$
The first two moments are quite trivial, but the second displays already all of the features of the general organization principles given in (13).

To summarize, we give a detailed description of the steps necessary for a measurement of the first moment of the reconstructed mass distribution. The procedure for higher moments should be obvious from this. For each of the detector resolution functions, calculate its first moment for various values of the true invariant mass \( s_T \). This gives the function \( P^1(s_T) \). Fit this function to a third order polynomial in \( (s_T - \bar{m}_D^2) \) and call the coefficients \( P^1_n \). The theoretical expression for the reconstructed moment is then obtained using Eq. (15) for \( N = 1 \) and using the theoretical expression for the \( \langle (s_T - \bar{m}_D^2)^n \rangle \) given in the Appendix.

For many applications the detector resolution function \( P(s_R - s_T, s_T) \) does not depend on the value of the true invariant mass and is therefore only a function of the difference of the true and the reconstructed mass

\[
P(s_R - s_T, s_T) = p(s_R - s_T).
\]

In this case, the expression in Eq. (15) simplifies considerably, since the quantities \( P^N_n \) can now be expressed solely in terms of moments of the resolution function. We find

\[
P^N_n = \binom{N}{n} p^{N-n},
\]

where \( p^N = \int ds s^n p(s) \). This allows to write an even simpler relations between the moment of the reconstructed and true spectra. For example, for the first moment

\[
\langle s_R - \bar{m}_D^2 \rangle = \langle s_T - \bar{m}_D^2 \rangle + p^1_{X} + (p^1_{D} - p^1_{X}) \frac{\Gamma_D}{\Gamma} + (p^1_{D'} - p^1_{X}) \frac{\Gamma_D'}{\Gamma},
\]

Note that Eq. (21) is exact, i.e., it does not contain unknown \( \sigma \Lambda^2_{QCD}/m_b^2 \) corrections as Eq. (15) does. In general, for the \( N \)-th moment of the reconstructed spectrum the first \( N \) moments of the resolution function, as well as the first \( N \) moments of the true spectrum are needed. For distributions with vanishing first moment, \( p^1 = 0 \), we see that the detector resolution function introduces no bias into the determination of the first moment of \( (s_T - \bar{m}_D^2) \). In practice, however, a detector always can miss particles and the first moments, \( p^1 \), are therefore expected to be negative.

To summarize, we have shown how to relate moments of the reconstructed hadronic invariant mass spectrum to the moments of the true, calculable, spectrum, involving only moments of the detector resolution functions.

We have given expressions for the general case, in which the resolution functions can depend on the true invariant mass, as well as for the special case, in which the resolution functions only depend on the difference between the true and the reconstructed invariant mass.

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**APPENDIX A: THE FIRST THREE HADRONIC MOMENTS**

In this appendix we give the expressions for the first hadronic moments \( S_n = \langle (s_T - \bar{m}_D^2)^n \rangle \) [note that this definition of \( S_n \) is slightly different than the one for \( \mathcal{M}_n \) in Eq. (2)]. Since the hadronic moments satisfy \( S_n \sim (\Lambda_{QCD}/m_b)^n \), the first three moments are non-vanishing to order \( 1/m_b^3 \). The decay rate \( \Gamma \), and the first two moments \( S_1 \), \( S_2 \) were calculated in the pole scheme as a function of the lepton energy cut in [2]. In [4] this calculation was repeated in several different mass schemes and explicit expressions were given for the dependence on the lepton energy cut. For completeness, we will repeat these results here and also give the result for the third moment \( S_3 \), which has not been presented in the literature so far. All these results are given in the 1S scheme, and for comparison with earlier works also in the pole scheme. They are written in the form

\[
S_n(E_0) = S_n^{(1)}(E_0) + S_n^{(2)}(E_0) \Lambda + S_n^{(3)}(E_0) \Lambda^2 + S_n^{(4)}(E_0) \Lambda^3 + S_n^{(5)}(E_0) \lambda_1 + S_n^{(6)}(E_0) \lambda_2 + S_n^{(7)}(E_0) \lambda_1 \lambda_2 + S_n^{(8)}(E_0) \lambda_2 \Lambda + S_n^{(9)}(E_0) \rho_1 + S_n^{(10)}(E_0) \rho_2 + S_n^{(11)}(E_0) T_1 + S_n^{(12)}(E_0) T_2 + S_n^{(13)}(E_0) T_3 + S_n^{(14)}(E_0) T_4 + S_n^{(15)}(E_0) \epsilon + S_n^{(16)}(E_0) \epsilon_{BLM} + S_n^{(17)}(E_0) \epsilon \Lambda,
\]

where \( E_0 \) is the value of the lepton energy cut, and the coefficients \( S_n^{(m)}(E_0) \) has the appropriate mass dimension. The parameter \( \epsilon \equiv 1 \) and \( \epsilon_{BLM} \equiv 1 \) denote the order in perturbation theory, for which we have used \( \alpha_s(m_b) = 0.22 \).
analytical results were given in \[2\]. Here we give the expressions for the additional moments needed to calculate the term with zero lepton energy cut.

These bremsstrahlung contributions were calculated in \[3\] with a cut on the lepton energy. However, virtual diagrams with corrections proportional to $\alpha$ \[0\] are shown in tables I to VI. The tables do not contain the $\Lambda$ pole in the Pole scheme as a function of $E_0$. For the first two hadronic invariant mass moments one needs the $\Lambda$ pole term with zero lepton energy cut $E_0$. This is because the radiative corrections to the hadronic energy distribution with a lepton energy cut are not known; for details see Ref. [3]. In Appendix B we give analytical expressions required for the $\Lambda$ term with zero lepton energy cut.

**APPENDIX B: ANALYTIC EXPRESSIONS FOR PERTURBATIVE CORRECTIONS TO NEW PARTONIC MOMENTS**

The leading perturbative corrections to the hadronic invariant moments arise only from bremsstrahlung contributions, since the virtual contributions are proportional to a $\delta$-function which does not contribute to the moments. These bremsstrahlung contributions were calculated in [3] with a cut on the lepton energy. However, virtual diagrams do contribute to perturbative corrections to the terms suppressed by powers of $\Lambda_{QCD}/m_b$. Using

$$s_H = m_B^2 + 2m_B m_b (\hat{s}_0 - 1) + m_b^2 (1 + \hat{s}_0 - 2 \hat{e}_0),$$  

the corrections proportional to $\alpha_s \Lambda_{QCD}/m_b$ can be obtained from the perturbative corrections to the partonic invariant mass $\hat{s}_0 = p_T^2/m_b^2$ and partonic energy $\hat{e}_0 = e_c/m_b$. For the first two hadronic invariant mass moments one needs the partonic moments $M^{(0,0)}, M^{(1,0)}, M^{(2,0)}, M^{(0,1)}, M^{(0,2)}$ and $M^{(1,1)}$, where we used the definition of \[2\]

$$M^{(n,m)} = \int d\hat{s}_0 d\hat{e}_0 \left(\hat{s}_0 - m_c^2\right)^n e_c^m m_b d\hat{s}_0 d\hat{e}_0,$$

with $m_c = m_c/m_b$. Perturbative corrections to these partonic moments can be obtained using the results of \[8\] and analytical results were given in \[2\]. Here we give the expressions for the additional moments needed to calculate the third hadronic invariant mass moments. Writing

$$M^{(n,m)} = M^{(n,m)}_{\text{non-pert}} + \frac{\alpha_s}{\pi} M^{(n,m)}_{\text{pert}},$$

and $\beta_0 = 25/3$. The definition of the parameter $\Lambda$ depends on the mass scheme used and is

$$\Lambda_{\text{pole}} = \tilde{m}_B - m_b^{\text{pole}} + \frac{\lambda_1}{2m_b} - \frac{\rho_1 - T_1 - T_2}{m_b^2}$$  

and

$$\Lambda^{18} = \frac{\tilde{m}_B}{2} - m_b^{18}.$$

The values for the coefficients $S_n^{(i)}$ are shown in tables I to VI. The tables do not contain the $\epsilon\Lambda$ term for non-zero lepton energy cut $E_0$. For the first two hadronic invariant mass moments one needs the $\Lambda$ pole term with zero lepton energy cut.
we find for the perturbative corrections

\[ M_{\text{pert}}^{(3,0)} = \frac{377}{132300} \hat{m}_c^2 + \frac{119}{2700} \hat{m}_c^4 + \frac{401}{900} \hat{m}_c^6 + \frac{97}{36} \hat{m}_c^8 + \frac{1}{12} \hat{m}_c^{10} - \frac{491}{900} \hat{m}_c^{12} - \frac{5531}{2700} \hat{m}_c^{14} - \frac{55747}{132300} \hat{m}_c^{16} \]

\[ + \left( \frac{16}{9} \hat{m}_c^6 + \frac{29}{9} \hat{m}_c^8 + \frac{3}{15} \hat{m}_c^{10} + \frac{7}{11} \hat{m}_c^{12} + \frac{11}{105} \hat{m}_c^{14} \right) \log(\hat{m}_c^2) \]

\[ M_{\text{pert}}^{(2,1)} = \frac{1081}{132300} \hat{m}_c^2 - \frac{187}{1350} \hat{m}_c^4 + \frac{637}{600} \hat{m}_c^6 + \frac{127}{216} \hat{m}_c^8 - \frac{1}{12} \hat{m}_c^{10} - \frac{259}{150} \hat{m}_c^{12} + \frac{25033}{264600} \hat{m}_c^{14} \]

\[ - \left( \frac{7}{12} \hat{m}_c^4 + \frac{12}{15} \hat{m}_c^6 + \frac{4}{15} \hat{m}_c^8 + \frac{1}{12} \hat{m}_c^{10} + \frac{13}{180} \hat{m}_c^{12} + \frac{13}{420} \hat{m}_c^{14} \right) \log(\hat{m}_c^2) \]

\[ M_{\text{pert}}^{(1,2)} = \frac{7421}{176400} + \frac{4079}{10800} \hat{m}_c^2 - \frac{341}{1200} \hat{m}_c^4 - \frac{71}{144} \hat{m}_c^6 - \frac{17}{48} \hat{m}_c^8 + \frac{257}{1200} \hat{m}_c^{10} - \frac{131}{1200} \hat{m}_c^{12} - \frac{53819}{529200} \hat{m}_c^{14} \]

\[ + \left( \frac{4}{15} \hat{m}_c^2 + \frac{13}{60} \hat{m}_c^4 + \frac{1}{12} \hat{m}_c^6 + \frac{17}{36} \hat{m}_c^8 + \frac{12}{15} \hat{m}_c^{10} + \frac{4}{105} \hat{m}_c^{12} \right) \log(\hat{m}_c^2) \]

\[ M_{\text{pert}}^{(0,3)} = \frac{289223}{1058400} + \frac{762659}{1058400} \hat{m}_c^2 - \frac{67337}{196000} \hat{m}_c^4 - \frac{52836}{529200} \hat{m}_c^6 - \frac{50705623}{392000} \hat{m}_c^8 + \frac{21613}{58800} \hat{m}_c^{10} \]

\[ - \frac{260423}{529200} \hat{m}_c^{12} + \frac{2}{4} \hat{m}_c^2 - \frac{499}{600} \hat{m}_c^4 + \frac{126121}{50400} \hat{m}_c^6 + \frac{8704}{105} \hat{m}_c^8 + \frac{57373}{2520} \hat{m}_c^{10} - \frac{667}{2520} \hat{m}_c^{12} \]

\[ + \log(\hat{m}_c^2) \left( \frac{1}{7} \hat{m}_c^2 - \frac{499}{5000} \hat{m}_c^4 + \frac{126121}{50400} \hat{m}_c^6 + \frac{8704}{105} \hat{m}_c^8 + \frac{57373}{2520} \hat{m}_c^{10} - \frac{667}{2520} \hat{m}_c^{12} \right) \]

\[ - \frac{257}{25200} \hat{m}_c^{14} - \frac{2743}{35280} \hat{m}_c^{16} - \log(1 - \hat{m}_c^2) \left( \frac{151}{882} + \frac{41}{225} \hat{m}_c^2 + \frac{5}{9} \hat{m}_c^4 + \frac{3}{2} \hat{m}_c^6 + \frac{3}{9} \hat{m}_c^8 + \frac{5}{9} \hat{m}_c^{10} - \frac{41}{225} \hat{m}_c^{12} \right) \]

\[ + \frac{151}{882} \hat{m}_c^{14} + \log(1 - \hat{m}_c^2) \left( \frac{3}{14} + \frac{7}{10} \hat{m}_c^2 + \frac{1}{2} \hat{m}_c^4 + \frac{1}{12} \hat{m}_c^6 - \frac{4352}{105} \hat{m}_c^8 - \frac{57373}{2520} \hat{m}_c^{10} - \frac{667}{2520} \hat{m}_c^{12} \right) \]

\[ + \frac{7}{10} \hat{m}_c^{14} + \hat{m}_c^8 \left( \frac{1}{7} + \frac{7}{10} \hat{m}_c^2 + \frac{3}{14} \hat{m}_c^4 + \frac{1}{12} \hat{m}_c^6 - \frac{4352}{105} \hat{m}_c^8 + \frac{57373}{2520} \hat{m}_c^{10} - \frac{667}{2520} \hat{m}_c^{12} \right) \]
TABLE V: Coefficients for $S_2(E_0)$ in the 1S scheme as a function of $E_0$.

| $E_0$ | $s_2^{(1)}$ | $s_2^{(2)}$ | $s_2^{(3)}$ | $s_2^{(4)}$ | $s_2^{(5)}$ | $s_2^{(6)}$ | $s_2^{(7)}$ | $s_2^{(8)}$ | $s_2^{(9)}$ | $s_2^{(10)}$ | $s_2^{(11)}$ | $s_2^{(12)}$ | $s_2^{(13)}$ | $s_2^{(14)}$ | $s_2^{(15)}$ | $s_2^{(16)}$ | $s_2^{(17)}$ |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0     | 0.816 3.188 3.889 1.73 | $-1.95$ | $-1.28$ | 5.06 | $-2.78$ | $-4.69$ | 0.67 | $-0.06$ | $-2.38$ | 0.77 | 0.1 | 0.454 | $-0.47$ | 0.356 |
| 0.5   | 0.795 3.106 3.784 1.68 | $-1.88$ | $-1.19$ | 5.08 | $-2.55$ | $-4.75$ | 0.57 | $-0.05$ | $-2.32$ | 0.76 | 0.11 | 0.469 | $-0.465$ | - |
| 0.7   | 0.77 3.005 3.651 1.61 | $-1.79$ | $-1.06$ | 5.13 | $-2.23$ | $-4.83$ | 0.43 | $-0.03$ | $-2.23$ | 0.76 | 0.13 | 0.499 | $-0.458$ | - |
| 0.9   | 0.738 2.872 3.471 1.5 | $-1.63$ | $-0.87$ | 5.24 | $-1.74$ | $-4.99$ | 0.24 | $-0.01$ | $-2.11$ | 0.75 | 0.16 | 0.562 | $-0.446$ | - |
| 1.1   | 0.702 2.722 3.258 1.37 | $-1.42$ | $-0.62$ | 5.48 | $-1.08$ | $-5.24$ | $-0.02$ | 0.03 | $-1.94$ | 0.74 | 0.2 | 0.678 | $-0.43$ | - |
| 1.3   | 0.668 2.572 3.031 1.2 | $-1.12$ | $-0.3$ | 5.94 | $-0.21$ | $-5.66$ | $-0.34$ | 0.08 | $-1.72$ | 0.74 | 0.26 | 0.888 | $-0.411$ | - |
| 1.5   | 0.641 2.45 2.826 1.03 | $-0.68$ | 0.11 | 6.9 | 0.98 | $-6.41$ | $-0.7$ | 0.17 | $-1.43$ | 0.76 | 0.34 | 1.302 | $-0.388$ | - |
| 1.7   | 0.638 2.423 2.746 0.92 | 0.13 | 0.72 | 9.27 | 2.84 | $-7.99$ | $-1.03$ | 0.35 | $-0.94$ | 0.82 | 0.47 | 2.295 | $-0.369$ | - |

TABLE VI: Coefficients for $S_3(E_0)$ in the 1S scheme as a function of $E_0$.

| $E_0$ | $s_3^{(1)}$ | $s_3^{(2)}$ | $s_3^{(3)}$ | $s_3^{(4)}$ | $s_3^{(5)}$ | $s_3^{(6)}$ | $s_3^{(7)}$ | $s_3^{(8)}$ | $s_3^{(9)}$ | $s_3^{(10)}$ | $s_3^{(11)}$ | $s_3^{(12)}$ | $s_3^{(13)}$ | $s_3^{(14)}$ | $s_3^{(15)}$ | $s_3^{(16)}$ | $s_3^{(17)}$ |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| 0     | 0.87 5.084 11.102 11.43 | $-9.59$ | $-2.52$ | $-12.73$ | $-10.45$ | 10.06 | 3.84 | $-1.51$ | $-7.75$ | 1.08 | 0.03 | 3.094 | 0.309 | 3.441 |
| 0.5   | 0.84 4.905 10.7 10.99 | $-9.26$ | $-2.34$ | $-12.05$ | $-9.68$ | 9.54 | 3.47 | $-1.45$ | $-7.5$ | 1.06 | 0.05 | 3.067 | 0.255 | - |
| 0.7   | 0.806 4.7 10.232 10.47 | $-8.85$ | $-2.12$ | $-11.14$ | $-8.7$ | 8.82 | 3. | $-1.38$ | $-7.18$ | 1.04 | 0.08 | 3.1 | 0.205 | - |
| 0.9   | 0.764 4.445 9.638 9.78 | $-8.29$ | $-1.81$ | $-9.8$ | $-7.31$ | 7.75 | 2.35 | $-1.28$ | $-6.76$ | 1.01 | 0.12 | 3.235 | 0.148 | - |
| 1.1   | 0.719 4.167 8.977 8.99 | $-7.61$ | $-1.43$ | $-8.02$ | $-5.55$ | 6.3 | 1.56 | $-1.16$ | $-6.26$ | 0.98 | 0.17 | 3.558 | 0.1 | - |
| 1.3   | 0.675 3.896 8.314 8.15 | $-6.83$ | $-0.96$ | $-5.68$ | $-3.38$ | 4.33 | 0.62 | $-1.02$ | $-5.7$ | 0.97 | 0.25 | 4.223 | 0.062 | - |
| 1.5   | 0.641 3.674 7.739 7.37 | $-5.94$ | $-0.38$ | $-2.43$ | $-0.6$ | 1.52 | $-0.47$ | $-0.84$ | $-5.09$ | 0.97 | 0.35 | 5.608 | 0.028 | - |
| 1.7   | 0.631 3.594 7.486 6.94 | $-4.75$ | 0.44 | 3.2 | 3.45 | $-3.39$ | $-1.76$ | $-0.58$ | $-4.35$ | 1.04 | 0.52 | 9.047 | $-0.01$ | - |

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