Open and hidden heavy flavour production (mostly in pp collisions): theory overview

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Two central aspects of the problem

- 1. What is the (structural) difference between open heavy-flavour(HF) meson and quarkonium?
 - ► For open HF mesons the "naive" quark model receives large corrections:

 $\left|D^{0}\right\rangle = c_{0}\left|(c\bar{u})_{1}\right\rangle + c_{1}\left|(c\bar{u})_{8}g\right\rangle + c_{2}\left|c\bar{u}d\bar{d}\right\rangle + \ldots, \ c_{0} \sim c_{1} \sim c_{2} \sim \ldots$

▶ For quarkonia (*we hope*) the more complicated Fock-states are suppressed by relative velocity (*v*) of heavy-quarks in the bound state

$$\begin{aligned} |J/\psi\rangle &= O(1) \left| c\bar{c} \left[{}^{3}S_{1}^{(1)} \right] \right\rangle + O(v) \left| c\bar{c} \left[{}^{3}P_{J}^{(8)} \right] + g \right\rangle \\ &+ O(v^{3/2}) \left| c\bar{c} \left[{}^{1}S_{0}^{(8)} \right] + g \right\rangle + O(v^{2}) \left| c\bar{c} \left[{}^{3}S_{1}^{(8)} \right] + gg \right\rangle + \dots, \end{aligned}$$

- 2. How heavy quark (or $Q\bar{Q}$ -pair) is produced in *pp*-collision? Collinear Factorization + pQCD. 3 regimes:
 - ▶ $p_T \sim M$, where *M* is the meson mass (~ m_Q or $2m_Q$). "fixed-order regime"
 - ▶ $p_T \gg M$, "fragmentation regime"
 - ▶ $p_T \ll M$, "TMD regime"

Open heavy-flavour hadron production

Open heavy flavours at $p_T \sim M$: fragmentation model

The p_T -spectrum of heavy quarks produced in pp-collisions can be computed up to NLO in α_s with available tools (MadGraph, Herwig, ...).

Transition from quark (\mathbf{p}_Q) momentum spectrum to hadron (\mathbf{p}) momentum, using fragmentation model:

$$\frac{d\sigma}{d^3\mathbf{p}} = \int_0^1 \frac{dz}{z^3} D_{\mathcal{H}/Q}(z) \frac{d\sigma_Q(\mathbf{p}_Q = p/z)}{d^3\mathbf{p}_Q},$$

where $D_{\mathcal{H}/Q}(z)$ – (scale-independent) fragmentation function for the hadron \mathcal{H} . Probability $B(Q \to \mathcal{H}_Q) = \int_0^1 dz D(z)$ and/or

 $\langle z \rangle = \int_{0}^{1} dz \ z D(z)$ is constrained from $e^{+}e^{-}$ data, e.g. [ALEPH, 01'] : $\langle z_{B} \rangle = 0.7361 \pm 0.0061.$

Several models for FFs are currently in use, e.g.:

• Peterson *et al.*: $D(z) = \frac{C}{z(1-\frac{1}{z}-\frac{\epsilon}{1-z})^2}, \ \epsilon_D \simeq 0.002 - 0.006$

► Kartvelishvili *et al.*: $D(z) = Cz^{\alpha}(1-z)$, $\alpha_D = 4.4 \pm 1.7$ (*D*-meson photoproduction), $\alpha_B = 11 \pm 4$ (*B*-mesons in e^+e^-).

Does this work?

PROSA PDF fit [Zenaiev et al., hep-ph/1503.04581], using massive NLO calculations for $c\bar{c}$ production [Nason et al. 88']. Kartvelishvili FFs with parameters fixed from e^+e^- data where used.



My doubts:

- If $m_{\mathcal{H}} \neq m_Q$ then it is not clear how to relate full four-momentum of quark and meson. Several prescriptions are possible. Important e.g. for pair production $m_{\mathcal{H}\mathcal{H}}, \Delta y,...$
- ▶ Not a factorisation "theorem" on any level of rigour for $p_T \sim M$. Are we sure that there is no way to do better in QCD? (LCDAs???)

NLO QCD calculation at $p_{TQ} \gg m_Q$

See e.g. [Kramer, 01'].

$$\frac{d\sigma_Q}{d^3\mathbf{p}_Q} = \int_0^1 dx_1 dx_2 f_i(x_1, \mu_F) f_j(x_2, \mu_F) \frac{d\hat{\sigma}_{ij}}{d^3\mathbf{p}_Q}(x_1, x_2),$$

at NLO for
$$|\mathbf{p}| \gg m_Q$$
:

$$\frac{d\hat{\sigma}_{ij}^{(\text{NLO})}}{d^{3}\mathbf{p}_{Q}} = \frac{d\hat{\sigma}_{ij}^{(\text{NLO},\text{ZML})}}{d^{3}\mathbf{p}_{Q}} + \frac{\alpha_{s}(\mu_{R})}{2\pi} \ln \frac{|\mathbf{p}_{Q}|^{2}}{m_{Q}^{2}} \sum_{k=q,g} \int_{0}^{1} \frac{dz}{z^{3}} P_{qk}(z) \left. \frac{d\hat{\sigma}_{ij\to k}^{(\text{LO})}}{d^{3}\mathbf{p}_{k}} \right|_{\mathbf{p}_{k}=\mathbf{p}_{Q}/z} + O\left(\frac{m_{Q}}{|\mathbf{p}_{Q}|}\right)$$

the remnant term is related to the massless NLO calculation with \overline{MS} -subtraction for FS-collinear divergence:

$$\frac{d\hat{\sigma}_{ij}^{(\text{NLO,ZML})}}{d^{3}\mathbf{p}_{Q}} = \frac{d\hat{\sigma}_{ij}^{(\text{NLO,m}_{Q}=0,\overline{\text{MS}})}}{d^{3}\mathbf{p}_{Q}} + \int_{0}^{1} \frac{dz}{z^{3}} d_{Q(m)/q(m=0)}(z) \left. \frac{d\hat{\sigma}_{ij\to q}^{(\text{LO})}}{d^{3}\mathbf{p}_{k}} \right|_{\mathbf{p}_{k}=\mathbf{p}_{Q}/z},$$
$$\hat{\sigma}_{ij}^{(\text{ZMLA})}$$
$$d_{Q(m)/q(m=0)}(z) = \frac{\alpha_{s}C_{F}}{2\pi} \left[\frac{1+z^{2}}{1-z} \left(-2\ln(1-z)-2\right) \right]_{+}.$$
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Resummation of fragmentation logs

Series of corrections $\alpha_s^n \ln^n \frac{|\mathbf{p}|}{m_Q}$ (LLA) can be resummed using DGLAP evolution of the fragmentation function:

$$\frac{d\hat{\sigma}_{ij}^{(\mathrm{LLA})}}{d^{3}\mathbf{p}_{Q}} = \sum_{k=q,g} \int_{0}^{1} \frac{dz}{z^{3}} D_{Q/k}(z,\mu_{F}) \left. \frac{d\hat{\sigma}_{ij\rightarrow q}^{(\mathrm{LO})}}{d^{3}\mathbf{p}_{k}} \right|_{\mathbf{p}_{k}=\mathbf{p}_{Q}/z},$$
$$\frac{dD_{i/k}(x,\mu_{F})}{d\ln\mu_{F}^{2}} = \frac{\alpha_{s}(\mu_{F})}{2\pi} \int_{x}^{1} \frac{dz}{z} P_{ij}(z) D_{j/k}\left(\frac{x}{z},\mu_{F}\right),$$

with initial conditions at $\mu_F = m_Q$:

$$D_{Q/q}^{(\text{LLA})}(z, m_Q) = \delta(1-z), \ D_{Q/g}(z, m_Q) = 0.$$

The corrections $\sim \alpha_s^{n+1} \ln^n \frac{|\mathbf{p}|}{m_Q}$ belong to NLLA:

$$D_{Q/q}^{(\text{NLLA})}(z, m_Q) = \delta(1-z) + d_{Q(m)/q(m=0)}(z),$$

as well as $P_{ij}(z)$ and $\hat{\sigma}_{ij\to k}$ @NLO \overline{MS} .

From quarks to hadrons: FONLL formalism

In the FONLL formula, the massive NLO quark production coefficient function is combined with the NLL resummed one using weight-function $G(p_T)$:



Then Kartvelishvili-type FF fitted to e^+e^- data is used to convert quarks to mesons. Typical results [Cacciari et al., 1205.6344] :



From quarks to hadrons: GM-VFNS

In the general-mass/variable flavour number scheme [Kramer 01'; Kniehl, Kramer, Schienbein, Speisberger 05'] the coefficient functions are computed as:

$$rac{\hat{\sigma}^{(\mathrm{GM-VFNS})}}{d^3\mathbf{p}} = rac{\hat{\sigma}^{(\mathrm{NLO})}_{ij}}{d^3\mathbf{p}} - rac{\hat{\sigma}^{(\mathrm{ZMLA})}_{ij}}{d^3\mathbf{p}},$$

so that they include mass effects and yet, the \overline{MS} PDFs and scale-dependent-FFs (fitted consistently using e^+e^- data) in the $n_F = n_{FL} + 1$ -scheme can be used at $p_T \gg m_Q$. Recent plots from [1907.12456] for B-Mesons:



$p_{T\mathcal{H}\mathcal{H}} \ll M_{\mathcal{H}\mathcal{H}}$, the TMD regime?

- ► The studies of $p_T \ll M$ regime of single-inclusive hadron production are not done, probably because they are poorly motivated theoretically $(M_H \sim 1 \text{ GeV after all...})$.
- ► For the **hadron-pair** production, one can have $p_{THH} \ll M_{HH}$ and $M_{HH} \gg \Lambda_{QCD}$! Heavy quark pair couples predominantly to gluons – excellent probe of gluon TMD PDFs and FFs ???
- ▶ Naively one can write the factorization fromula of the type:

$$\frac{d\sigma}{d^2 \mathbf{p}_{T\mathcal{H}\mathcal{H}}} \propto \int d^2 \mathbf{q}_{T1} d^2 \mathbf{q}_{T2} d^2 \mathbf{k}_{T1} d^2 \mathbf{k}_{T2} f_g(x_1, \mathbf{q}_{T1}) f_g(x_2, \mathbf{q}_{T2}) D(z_1, \mathbf{k}_{T1}) D(z_1, \mathbf{k}_{T2}) \\ \times \delta^{(2)}(\mathbf{q}_{T1} + \mathbf{q}_{T2} + \mathbf{k}_{T1} + \mathbf{k}_{T2} - \mathbf{p}_{T\mathcal{H}\mathcal{H}}),$$

and declare it to be true up to corrections $O(|\mathbf{p}_{T\mathcal{H}\mathcal{H}}|/M_{\mathcal{H}\mathcal{H}})$, following analogy with Drell-Yan and SIDIS processes. The TMD FFs can be extracted from e^+e^- data, so constraining the TMD PDFs becomes possible?

Factorization violation

Arguments against such factorization are given in [Collins, Qiu, 07'; Rogers, Mulders, 10']:

- ▶ Factorization theorems are proven in perturbation theory just as universal structure of expansion of some quantity in the relevant limit $(|\mathbf{p}_{T\mathcal{H}\mathcal{H}}|/M_{\mathcal{H}\mathcal{H}} \ll 1 \text{ in this case})$ up to power-suppressed corrections. The theorems should not depend on detailed assumptions on the structure of colliding objects, therefore model calculations can be used to (in-)validate them.
- The argument starts by disproving the factorization structure of transverse single-spin asymmetry. The TSSA in the model comes from 3 types of diagrams (because they give Im parts):



▶ Suppose colliding (dashed) partons have different flavours with different couplings to (Abelian) gluons: g_1 and g_2 . Then the first diagram can be considered as the contribution of (Sievers) TMD PDF of the 1st hadron, but the second and third – can not. 11/2

Factorization violation

▶ To obtain the contribution of this mechanism to the spin-averaged cross section, one needs to square the imaginary part, i.e. to add the gluon exchange:



- Contributions of this kind could not be put into TMD PDF of the first hadron in a theory with two couplings g_1 and g_2 and hence violate "naive" TMD factorization with process-independent TMD PDFs.
- ▶ Detailed calculation in QCD with one coupling confirms that these contribution does not cancel, so it is not an artifact of $g_1 \neq g_2$. QED.
- Later attempts to modify factorization by giving-up process-independence of TMD PDFs just pushed the problem one order in α_s higher [Rogers, Mulders, 10].

My (vague) thoughts:

- ▶ Does this all apply to the process $gg \rightarrow Q\bar{Q}$? Maybe m_Q -suppressed?
- All arguments for σ_{unpol}, so far look like Δσ_{unpol} ~ Im². Does this mean that FV can be estimated from observables sensitive to Im parts, like TSSA, and is bound to be very small?

PHENIX results for light hadrons





The distribution width increases (logarithmically?) with p_T of single hadron, similarly to what CSS evolution of TMD PDFs would give.

How this picture looks like for heavy hadrons? At higher energies?

Quarkonium production

Quarkonium in the potential model

Cornell potential:

$$V(r) = -C_F \frac{\alpha_s(1/r)}{r} + \sigma r,$$

neglect linear part, because quarkonium is "small" ($\sim 0.3 \text{ fm}$) \rightarrow Coulomb wavefunction (for effective mass $\frac{m_1m_2}{m_1+m_2} = \frac{m_Q}{2}$): αs²(m_{Q*}v) 0.5 0.4 $R(r) = \frac{\sqrt{m_Q^3 \alpha_s^3 C_F^3}}{2} e^{\frac{1}{2}}$ n_=1.5 Ge 0.3 $\langle v^2 \rangle = \frac{C_F^2 \alpha_s^2}{2}, \langle r \rangle = \frac{3}{2C_F} \frac{1}{m_O v}$ 0.2 mb=4.8 GeV $\Rightarrow \alpha_s^2(m_Q v) \simeq v^2$ 0.1 ⊥ v² 0.0 0.1 0.2 0.3 04 0.5

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Does hydrogen atom contain photons?

Yes, if we couple Schrödinger bound-state problem to the dynamical E-M field:

$$\hat{H} = \hat{H}_{\text{at.}} + \hat{H}_{\text{EMF}} + \hat{H}_{\text{E-dip.}} + \hat{H}_{\text{M-dip.}} + \dots,$$
$$\hat{H}_{\text{at.}} = -\frac{\nabla^2}{2m} + V(\hat{\mathbf{r}}), \hat{H}_{\text{E-dip.}} = e\hat{\mathbf{E}}(0) \cdot \hat{\mathbf{r}},$$
$$\hat{H}_{\text{M-dip}} = \frac{e\hbar}{2mc}\hat{\mathbf{H}}(0) \cdot [g_s\hat{\mathbf{S}} + \hat{\mathbf{r}} \times \hat{\mathbf{p}}].$$

and consider the electric-dipole interaction as perturbation over eigenstates of atom not coupled to EM field:

$$\hat{H}_{\mathrm{at.}}\left|n,L,L_{z},S_{z}\right\rangle = E_{n,L}\left|n,L,L_{z},S_{z}\right\rangle,$$

the first order of PT for ground state of \hat{H} :

$$\begin{aligned} |\mathbf{H} - \mathbf{a} \mathbf{t} \mathbf{o} \mathbf{n} \rangle &= |0, 0, 0, S_z\rangle |0\rangle + \\ e \sum_{n=1}^{\infty} |n, 1, \pm 1, S_z\rangle |\gamma\rangle \frac{\langle \gamma | \langle n, 1, \pm 1, S_z | \hat{\mathbf{r}} \cdot \hat{\mathbf{E}}(0) | 0, 0, 0, S_z\rangle |0\rangle}{E_{0,0} - E_{n,1} - E_{\gamma}} + \dots \end{aligned}$$

The corresponding correction to energy gives us the Lamb shift $_{\rm [Bethe,\ 47']}$.

Non-relativistic QCD

The velocity-expansion for quarkonium eigenstate is carbon-copy of corresponding arguments from atomic physics (hierarchy of E-dipole/M-dipole with ΔS /M-dipole transitions):

$$\begin{aligned} |J/\psi\rangle &= O(1) \left| c\bar{c} \left[{}^3S_1^{(1)} \right] \right\rangle + O(v) \left| c\bar{c} \left[{}^3P_J^{(8)} \right] + g \right\rangle \\ &+ O(v^{3/2}) \left| c\bar{c} \left[{}^1S_0^{(8)} \right] + g \right\rangle + O(v^2) \left| c\bar{c} \left[{}^3S_1^{(8)} \right] + gg \right\rangle + \dots, \end{aligned}$$

for validity of this arguments, we should work in *non-relativistic EFT*, dynamics of which conserves number of heavy quarks. In such EFT, $Q\bar{Q}$ -pair is produced in a point, by local operator:

$$\mathcal{A}_{\text{NRQCD}} = \langle J/\psi + X | \chi^{\dagger}(0) \kappa_n \psi(0) | 0 \rangle,$$

Different operators "couple" to different Fock states:

$$\chi^{\dagger}(0)\psi(0) \leftrightarrow \left| c\bar{c} \begin{bmatrix} {}^{1}S_{0}^{(1)} \end{bmatrix} \right\rangle, \ \chi^{\dagger}(0)\sigma_{i}\psi(0) \leftrightarrow \left| c\bar{c} \begin{bmatrix} {}^{3}S_{1}^{(1)} \end{bmatrix} \right\rangle,$$
$$\chi^{\dagger}(0)\sigma_{i}T^{a}\psi(0) \leftrightarrow \left| c\bar{c} \begin{bmatrix} {}^{3}S_{1}^{(8)} \end{bmatrix} \right\rangle, \ \chi^{\dagger}(0)D_{i}\psi(0) \leftrightarrow \left| c\bar{c} \begin{bmatrix} {}^{1}P_{1}^{(8)} \end{bmatrix} \right\rangle, \dots$$

squared NRQCD amplitude (=LDME):

$$\sum_{X} |\mathcal{A}|^{2} = \langle 0| \underbrace{\psi^{\dagger} \kappa_{n}^{\dagger} \chi a_{J/\psi}^{\dagger} a_{J/\psi} \chi^{\dagger} \kappa_{n} \psi}_{\mathcal{O}_{n}^{J/\psi}} |0\rangle = \left\langle \mathcal{O}_{n}^{J/\psi} \right\rangle,$$

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Non-relativistic QCD

Velocity-scaling of LDMEs follows from velocity-scaling of corresponding Fock states and of operators $\chi^{\dagger}\kappa_n\psi$:



$$v \to 0: \mathcal{A}_{\text{QCD}}(gg \to Y_{Q\bar{Q}(v)}) = \sum_{n} f_n \left\langle Y_{Q\bar{Q}(v)} \right| \chi^{\dagger}(0) \kappa_n \psi(0) \left| 0 \right\rangle + O(v^{\#}),$$

 \Rightarrow NRQCD factorization formula ("theorem") [Bodwin, Braaten, Lepage 95']:

$$\sigma(gg \to \mathcal{H} + X) = \sum_{n} \sigma(gg \to Q\bar{Q}[n] + X) \left\langle \mathcal{O}_{n}^{\mathcal{H}} \right\rangle.$$

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NRQCD factorization: what does work?

- Includes colour-singlet model for S-wave states as LO of velocity expansion
- ▶ Solves the problem of non-cancelling IR divergence at NLO in CSM for *P*-wave states production and decay through mixing with ${}^{3}S_{1}^{(8)}$ or ${}^{1}S_{0}^{(8)}$ states at $O(v^{2})$.
- ▶ Covers the gap between CSM (@LO and NLO) and data at high- p_T in hadroproduction, due to contribution of CO states. If

NNLO corrections in CS are as large as needed to close this gap, then perturbative expansion is

just useless and we should stop doing quarkonia.



· Data fitted to is described within scale uncertainties, other observables not.

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• Data fitted to is described, other observables not.



• Data fitted to is described, other observables not.



• Nontrivial: Largely unpolarized J/ ψ compatible with data (although tensions to CDF data). But: J/ ψ hadroproduction $p_T < 7$ GeV, J/ ψ photo- and J/ $\psi + Z$ production not described.



 Compared to Chao et al. fit on previous slide: Even better description of η_c production, at the expense of introducing also tensions with other determinations of <0^{1/ψ}(³S₁⁽¹⁾)>.

NRQCD factorization "puzzles"

Overall situation:

LDMEs	J/ψ hadropr.	J/ψ photopr.	J/ψ polar.	η_c hadropr.
Butenschön et al.	 Image: A set of the set of the	 Image: A set of the set of the	×	×
Chao et al. + η_c	 Image: A set of the set of the	×	1	 Image: A set of the set of the
Zhang et al.	1	×	1	 Image: A set of the set of the
Gong et al.	1	×	1	×
Chao et al.	1	×	1	×
Bodwin et al.	 Image: A set of the set of the	×	1	×

Puzzles:

- ▶ No way to describe J/ψ polarization in pp collisions and photoproduction data simulataneously "polarization puzzle"
- ▶ No way to reconcile HQSS relations between J/ψ and η_c LDMEs with J/ψ -photoproduction description "HQSS puzzle"
- However consistent description of hadroproduction alone is possible! And it is also a puzzle...
- ► Bulk of double- J/ψ production cross section seems to be well understood in terms of just double ${}^{3}S_{1}^{(1)}$ contribution, while $J/\psi + Z$ production is a mystery...

(Improved-)colour-evaporation model

"Fock-state-democratic" version of the colour-octet mechanism. All spin, colour and orbital momentum states contribute to quarkonium with the same probability if their invariant mass is between $2m_c$ or $M_{J/\psi}$ and $2m_D$:

$$\hat{\sigma}(gg \to J/\psi + X) = F_{J/\psi} \times \int_{M_{J/\psi}}^{2m_D} dM_{Q\bar{Q}} \frac{d\hat{\sigma}}{dM_{Q\bar{Q}}} (gg \to Q\bar{Q} + X)$$

- ► Can be extended to NLO for $\hat{\sigma}$ of $Q\bar{Q}$ -production
- ▶ Describes single-inclusive p_T -spectra, with some overshoot at high p_T
- Fails to describe the bulk of J/ψ-pair production by factor of 10 - 100 [Lansberg et.al., 20']
- ► Reasonably describes J/ψ polarisation in pp at high- p_T [Vogt, Chung]
- ► At LO has very strong $z \to 1$ peak for J/ψ photoproduction, inconsistent with data, needs ad-hoc tricks to remove it [Halsen]

Fragmentation approach to quarkonium production

- ▶ p_T -spectra for partonic production subprocesses of different Fock-states at LO have very different p_T -scaling for $p_T \gg M$: ~ $1/p_T^8$ for ${}^3S_1^{(1)}$ vs. $1/p_T^4$ for ${}^3S_1^{(8)}$. This hierarchy is removed by radiative corrections.
- At sufficiently high order in α_s all Fock-states can be produced with $\sim 1/p_T^4$ behaviour (Leading power).
- ▶ LP fragmentation formalism is well-known: the FFs at $\mu_F = M$ can be computed perturbatively in terms of LDMEs
- ► NLP fragmentation formalism also has been developed recently [Kang, Qiu, Sterman, 11']

TMD factorization for heavy quarkonia?

Due to ${}^{1}S_{0}^{(1)}$ -dominance of the η_{c} -production at small p_{T} , the factorization violation arguments for hadron-pair production are not valid for this state ?! But TMD factorization for the $p_{T} \ll M$ regime of η_{c} production is not simple. It includes new object – **TMD shape function** [Echevaria, 19'; Fleming, Makris, Mehen, 19']:

$$S(\mathbf{b}_T) = \langle 0 | \psi^{\dagger}(\mathbf{b}_T) \kappa_n^{\dagger} \chi(\mathbf{b}_T) a_{J/\psi}^{\dagger} a_{J/\psi} \chi^{\dagger}(0) \kappa_n \psi(0) | 0 \rangle,$$

where transverse coordinate \mathbf{b}_T is Fourier-conjugate to the transverse momentum (\mathbf{k}_T) of the $Q\bar{Q}$ -pair in the quarkonium, relative to the "light cloud".

My worry: the radius of quarkonium WF is ~ 0.3 fm against radius of the proton ~ 1 fm. Does it mean that $\langle k_T \rangle_{J/\psi} \sim 3\langle q_T \rangle_p$? If so, then what we study in the J/ψ pair production: structure of the proton or quarkonium?