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# Estimating the production rate of loosely bound hadronic molecules using event generators

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### Estimating the Production Rate of Loosely-bound Hadronic Molecules using Event Generators

Pierre Artoisenet and Eric Braaten Physics Department, Ohio State University, Columbus, Ohio 43210, USA (Dated: October 27, 2010)

We examine the use of hadronic event generators, such as Pythia or Herwig, to estimate the production rate of loosely-bound hadronic molecules, such as the deuteron and the X(3872). In the case of the deuteron, we point out that there are large uncertainties in the normalization of the predictions using event generators, because baryon pair distributions are not among the inputs used to tune the event generators. Predictions using Pythia for anti-deuteron production in  $\Upsilon$  decay are compared to measurements by the CLEO Collaboration. They suggest that Pythia overpredicts the probability of producing pairs of baryons, at least in  $\Upsilon$  decay into three gluons, and that the standard value of the coalescence parameter underpredicts the probability for formation of a deuteron from a neutron and proton with small relative momentum. In the case of the X(3872), we discuss a proposed upper bound on the prompt cross section at the Tevatron that has been used as an argument against the X(3872) being a loosely-bound charm meson molecule. We demonstrate that this proposed upper bound is invalid by showing that the analogous upper bound for the anti-deuteron would be smaller than the observed anti-deuteron cross section.

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## I. INTRODUCTION

Quantum mechanics predicts that a bound state that is sufficiently close to a 2-body threshold and that couples to that threshold through a short-range S-wave interaction has universal properties that depend only on its binding energy. Such a bound state is necessarily a loosely-bound molecule in which the constituents are almost always separated by more than the range. One of the universal predictions is that the root-mean-square (rms) separation of the constituents is  $(4\mu E_X)^{-1/2}$ , where  $E_X$  is the binding energy of the resonance and  $\mu$  is the reduced mass of the two constituents. As the binding energy is tuned to zero, the size of the molecule increases without bound. A classic example of a loosely-bound S-wave molecule is the deuteron, which is a bound state of the proton and neutron with binding energy 2.2 MeV. The proton and neutron are correctly predicted to have a large rms separation of about 3.1 fm.

An even more ideal example of a loosely-bound S-wave molecule is the charmonium-like state X(3872), provided that its  $J^{PC}$  quantum numbers are 1<sup>++</sup>. Measurements of its mass in the decay mode  $J/\psi \pi^+\pi^-$  indicate that it is below the threshold for  $D^{*0}\bar{D}^0$  by  $0.42\pm0.39$  MeV [1–4]. If its quantum numbers are 1<sup>++</sup>, it has an S-wave coupling to  $D^{*0}\bar{D}^0$ . In that case, it must be a loosely-bound molecule whose constituents are the superposition  $D^{*0}\bar{D}^0 + D^0\bar{D}^{*0}$ . The constituents are predicted to have a large rms separation of  $4.9^{+13.4}_{-1.4}$  fm.

The production rate of a deuteron or anti-deuteron in high energy collisions is an important problem for several reasons. Anti-deuterons can be produced by the annihilation or decay of very massive dark-matter particles. Thus they provide a low-background channel for the indirect detection of dark matter [5]. The production of deuterons and anti-deuterons has been observed in relativistic heavy ion collisions [6, 7]. Their production serves as a probe of the expanding and cooling hadronic fluid at the time of its freeze-out into free-streaming hadrons. The production of an anti-deuteron has also been observed in many high energy physics experiments, including  $\Upsilon$  decays [8, 9],  $p\bar{p}$  collisions [10], photoproduction [11],  $Z^0$  decays [12], and deep inelastic electron scattering [13]. To explain the production rate quantitatively in these experiments is a challenge. The production rate of the X(3872) is important for understanding the nature of some of the new  $c\bar{c}$  mesons above the open charm threshold that have been discovered in recent years [14]. Thus far, the X(3872) has been observed prompt production rate of the X(3872) at the Tevatron is orders of magnitude too large to be compatible with its identification as a loosely-bound S-wave molecule [15]. A subsequent analysis challenged this conclusion [16]. The resolution of the controversy has important implications for studies of the X(3872) in experiments at the Large Hadron Collider.

Estimating the production rate of a loosely-bound S-wave molecule in high energy collisions is also an interesting problem. Intuitively, one expects the cross section to be very small, because one would expect the binding of the constituents into a molecule to be easily disrupted by the enormous energies available in a high energy collision. On the other hand, since the constituents of the molecule are almost always outside the range of their interactions, they must be subject to a very strong force during the small fraction of time in which they are close together. This strong force also operates between constituents that are produced with small relative momentum in a high energy collision. The production rate of the molecule involves the interplay between this very strong force and the very weak binding.

One tool that can be helpful in estimating the production rate of a loosely-bound S-wave hadronic molecule is a hadronic event generator, such as Pythia [17] or Herwig [18]. These event generators can be interpreted as purely phenomenological models for hadron production with numerous parameters that have been adjusted to fit data from many high energy physics experiments. They should provide accurate predictions for observables that are sufficiently similar to the ones that have been used to tune the parameters, but one should be wary of applying them to new phenomena. They may be able to take into account the effects of generic hadronic interactions, but they should not be expected to take into account the effects of finely-tuned interactions, such as those responsible for the existence of loosely-bound hadronic molecules. Event generators have been used to estimate the production rate of anti-deuterons in the annihilation of dark-matter particles [19]. They have also been applied to the production rate of the X(3872) in hadron colliders [15, 16, 20].

In this paper, we address some of the issues involved in using hadronic event generators to estimate the production rate of loosely-bound S-wave hadronic molecules. In Section II, we discuss the use of an event generator to estimate the production rate of the anti-deuteron. In Section III, we compare measurements of anti-deuteron production in  $\Upsilon$ decays by the CLEO Collaboration with predictions from an event generator. In Section IV, we discuss the controversy involving the use of event generators to estimate the prompt production rate of the X(3872). We discuss our results in Section V.

#### **II. EVENT-GENERATOR MODEL FOR DEUTERON PRODUCTION**

The coalescence model is a purely phenomenological model for deuteron and anti-deuteron production [21]. According to this model, the differential distribution for a deuteron of momentum  $\boldsymbol{P}$  is the product of the differential distributions for a neutron and a proton with equal momenta  $\frac{1}{2}\boldsymbol{P}$  multiplied by a Lorentz boost factor  $E/2m_N$  and by a phenomenological constant. That constant is often expressed as the volume  $4\pi p_0^3/3$  of a sphere in momentum space. The coalescence model can be "derived" from two assumptions:

- 1. A neutron and a proton will bind to form a deuteron if they are produced with relative momentum less than  $p_0$ .
- 2. The joint probability distribution for producing n and p factors into the product of independent probabilities for n and p.

From an analysis of data on anti-deuteron production in proton-proton and proton-nucleus collisions with nucleonnucleon center-of-mass energies in the range 20 to 53 GeV, the coalescence parameter has been determined to be  $p_0 = 79$  MeV [22]. We will use  $p_0 = 80$  MeV to avoid the implication that this parameter can be determined with two digits of accuracy. We will refer to this value as the *standard coalescence parameter* for the deuteron.

Kadastik, Raidal, and Strumia recently pointed out that the coalescence model fails dramatically for the production of anti-deuterons in the annihilation of a pair of heavy dark-matter particles [19]. It predicts incorrectly that the probability for producing an anti-deuteron scales as  $1/M^2$ , where M is the mass of the dark-matter particle. However the probability is actually a slowly varying function of M. The reason the coalescence model fails is that a pair of dark-matter particles annihilates predominantly into two jets, and the  $\bar{d}$  is almost always produced by the coalescence of  $\bar{n}$  and  $\bar{p}$  within the same jet. While the separate probability distributions for  $\bar{n}$  and  $\bar{p}$  are spherically symmetric, the joint probability distribution for  $\bar{n}$  and  $\bar{p}$  is sharply peaked for  $\bar{n}$  and  $\bar{p}$  in the same direction. Thus assumption 2 of the coalescence model breaks down completely.

Kadastik, Raidal, and Strumia proposed an alternative model for the production of anti-deuterons that gives the correct scaling behavior when the production is dominated by jets [19]. They retained assumption 1, but assumption 2 was replaced by an alternative assumption:

2'. The joint probability distribution for producing n and p can be calculated using a hadronic event generator, such as Pythia or Herwig.

The model consisting of assumptions 1 and 2' implies a simple equation for the inclusive deuteron cross section:

$$\sigma[d] = \sigma_{\text{naive}}[np(k < p_0)]. \tag{1}$$

The subscript "naive" on the right side refers to the np cross section being calculated using a method that is not informed about the fine-tuning of interactions that is responsible for binding the n and p into d. In Ref. [19], the

authors used this model to calculate the  $\bar{d}$  yield per dark-matter annihilation event for various pairs of jets, using Pythia as their event generator. For a dark-matter particle with a mass M of about 100 GeV, the yields are larger than those predicted by the coalescence model by more than an order of magnitude and the discrepancy increases like  $M^2$ .

It should be obvious from its formulation that this model is a purely phenomenological model with no fundamental justification. However this model also has a practical problem in that it relies on Pythia or Herwig to give the distribution for pairs of baryons. Measurements of single-baryon momentum distributions in various high energy physics experiments have been used to tune these event generators, but, to the best of our knowledge, information about baryon pairs has not been used. Thus one should allow at least for an unknown normalizing factor  $K_{np}$  in its predictions for np pair distributions. This can be expressed as an alternative to the assumption 2 of the event-generator model:

2". The joint probability distribution for producing n and p can be calculated using a hadronic event generator, such as Pythia or Herwig, up to a normalizing factor  $K_{np}$ .

The model consisting of assumptions 1 and 2'' implies a simple equation for the inclusive deuteron cross section:

$$\sigma[d] = K_{np} \ \sigma_{\text{naive}}[np(k < p_0)]. \tag{2}$$

We will refer to this model as the *event-generator model*.

In the spirit of hadronic event generators, the normalizing factor  $K_{np}$  and the coalescence parameter  $p_0$  should be treated as phenomenological parameters that must be determined from data. Their values need not be the same in all high energy physics processes. Their values for large transverse momentum processes, which are dominated by jets, could be different from their values for low transverse momentum processes. They could have different values for processes initiated by quarks and antiquarks than for processes initiated by gluons. In the absence of data that can be used to determine  $p_0$  and  $K_{np}$  separately, the most reliable predictions of the event-generator model will be for ratios of observables in which  $K_{np}$  cancels.

The ALEPH Collaboration has measured the inclusive decay rate of the  $Z^0$  into an anti-deuteron [12]. The number of anti-deuterons per hadronic  $Z^0$  decay is

$$\frac{\mathcal{B}[Z^0 \to \bar{d} + X]}{\mathcal{B}[Z^0 \to \text{hadrons}]} = (5.9 \pm 1.8 \pm 0.5) \times 10^{-6}.$$
(3)

In Ref. [19], the production rate of  $\bar{d}$  in  $Z^0$  decay was calculated using the Pythia event generator. Taking the measurement in Eq. (3) as the input, the coalescence parameter was determined to be  $p_0 = 81 \pm 9$  MeV. This is consistent to within errors with the standard value  $p_0 = 80$  MeV. In the event-generator model, the branching ratio in Eq. (3) is sensitive only to the combination  $K_{np}p_0^3$ . Hadronic decays of the  $Z^0$  are dominated by its decay into a quark and antiquark, each of which hadronizes into a jet. Thus a conservative conclusion from the calculation in Ref. [19] is that  $K_{np}p_0^3 \approx (80 \text{ MeV})^3$  for  $\bar{d}$  production in a jet initiated by a quark or antiquark.

#### III. ANTI-DEUTERON PRODUCTION IN $\Upsilon$ DECAYS

The high energy process for which there is the most information about anti-deuteron production is  $\Upsilon$  decay. In this section, we compare measurements of anti-deuteron production in  $\Upsilon$  decay by the CLEO Collaboration [9] with predictions of the event-generator model.

#### A. CLEO measurements

The CLEO Collaboration has studied the production of the deuteron and the anti-deuteron in a data sample of  $2.2 \times 10^7 \Upsilon(1S)$  decays [9]. The rates for the deuteron and anti-deuteron are presumably equal, but the backgrounds are smaller for the anti-deuteron, because the CLEO detector is made of matter rather than antimatter. They also studied the production of the anti-deuteron  $\bar{d}$  in  $e^+e^-$  annihilation off the resonance. In  $e^+e^-$  annihilation, the production process is initiated by the decay of a virtual photon into a light quark-antiquark pair. In  $\Upsilon$  decay, the production process is initiated either by the annihilation of  $b\bar{b}$  into a virtual photon, which then decays into a light  $q\bar{q}$  pair, or by the direct annihilation of  $b\bar{b}$  into partons, such as 3 gluons. The virtual-photon contributions to the inclusive partial width of  $\Upsilon$  into  $\bar{d}$  and to the total hadronic width of  $\Upsilon$  can both be determined from measurements off the resonance. CLEO therefore found it convenient to express their results in terms of the "direct" branching

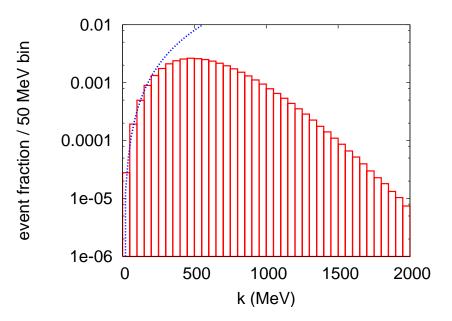


FIG. 1: Fraction of  $\Upsilon \to ggg$  events generated by Pythia with an  $\bar{n}\bar{p}$  pair in the final state as a function of the relative momentum k between the  $\bar{n}$  and  $\bar{p}$ . The dotted line is a phase space distribution proportional to  $k^2$ .

fraction, in which the virtual-photon contributions have been subtracted from both the numerator and denominator. Their result for the direct branching fraction was

$$\mathcal{B}^{\rm dir}[\Upsilon \to \bar{d} + X] = (3.36 \pm 0.23 \pm 0.25) \times 10^{-5}.$$
(4)

One can interpret this as the inclusive branching fraction into  $\bar{d}$  from the annihilation of  $\Upsilon$  into 3 gluons. For  $\bar{d}$  production from the decay of a virtual photon, CLEO set an upper bound on the inclusive branching fraction of about  $10^{-5}$ . Thus the production rate of  $\bar{d}$  is significantly larger in gluon-initiated processes than in  $q\bar{q}$ -initiated processes.

The presence of the anti-deuteron in an  $\Upsilon$  decay event implies that the event also includes at least two baryons. The CLEO Collaboration studied the nature of the associated baryons. Their results were consistent with the  $\bar{d}$  being accompanied by nn, np, and pp with probabilities 25%, 50%, and 25%, respectively. They also found 3 events out of their 338  $\bar{d}$  candidates in which the  $\bar{d}$  was accompanied by a d. The ratio of these numbers of events provides an estimate of the branching ratio for inclusive  $\bar{d} + d$  and inclusive  $\bar{d}$ :

$$\frac{\mathcal{B}^{\text{dir}}[\Upsilon \to \bar{d} + d + X]}{\mathcal{B}^{\text{dir}}[\Upsilon \to \bar{d} + X]} \approx 0.009.$$
(5)

The naive assumption that N events can have fluctuation of  $\pm \sqrt{N}$  implies that the error bar is at least as large as  $\pm 0.006$ .

#### B. Event-generator model

The event-generator model can be used to predict the production rate of an anti-deuteron from the annihilation of  $\Upsilon$  into 3 gluons. We have generated  $140 \times 10^6 \Upsilon \rightarrow ggg$  events using Pythia. The fraction of  $\Upsilon \rightarrow ggg$  events that include an  $\bar{n}\bar{p}$  pair is displayed in Figure 1 as a function of the relative momentum k between the  $\bar{n}$  and  $\bar{p}$ . The fraction of events follows a phase space distribution proportional to  $k^2$  out to about 200 MeV. We can therefore use the phase space distribution to calculate the fraction of  $\bar{n}\bar{p}$  events with  $k < p_0$ . The prediction of the event-generator model for the direct branching fraction into  $\bar{d}$  is

$$\mathcal{B}^{\rm dir}[\Upsilon \to \bar{n}\bar{p}(k < p_0) + X] = 1.1 \times 10^{-4} K_{np} \left(\frac{p_0}{80 \text{ MeV}}\right)^3.$$
(6)

If we set  $K_{np} = 1$  and  $p_0 = 80$  MeV, this prediction is larger than the CLEO measurement of the direct branching fraction in Eq. (4) by about a factor of 3.5.

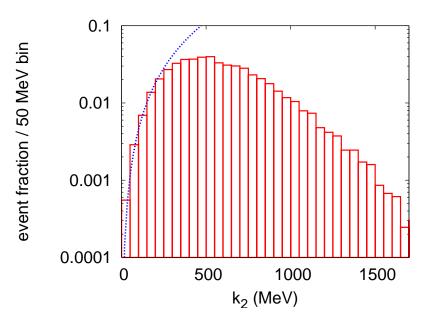


FIG. 2: Fraction of  $\Upsilon \to ggg \to \bar{n}\bar{p}(k_1 < 80 \text{ MeV}) + X$  events generated by Pythia with an np pair in the final state as a function of the relative momentum  $k_2$  between the n and p. The dotted line is a phase space distribution proportional to  $k_2^2$ .

The production of inclusive  $\bar{d} + d$  events can be studied in the event-generator model by counting the events with both an  $\bar{n}\bar{p}$  pair and an np pair, each of which has relative momentum smaller than  $p_0$ . The fraction of  $\Upsilon \to ggg \to \bar{n}\bar{p}(k_1 < p_0) + X$  events that include an np pair in the final state as a function of the relative momentum  $k_2$  between n and p is shown in Fig. 2. The fraction of events follows a phase space distribution proportional to  $k_2^2$ out to about 200 MeV. We can therefore use the phase space distribution to calculate the fraction of np events with  $k_2 < p_0$ . The prediction of the event-generator model for the ratio of the direct branching fractions into  $\bar{d} + d$  and  $\bar{d}$  is

$$\frac{\mathcal{B}^{\text{dir}}[\Upsilon \to \bar{n}\bar{p}(k_1 < p_0) + np(k_2 < p_0) + X]}{\mathcal{B}^{\text{dir}}[\Upsilon \to \bar{n}\bar{p}(k_1 < p_0) + X]} = 1.6 \times 10^{-3} \left(\frac{p_0}{80 \text{ MeV}}\right)^3.$$
(7)

The numerator is proportional to a single factor of  $K_{np}$ , because the presence of the  $\bar{n}\bar{p}$  pair requires an accompanying antibaryon pair. Thus the normalizing factor  $K_{np}$  cancels between the numerator and denominator. If we set  $p_0 = 80$  MeV in Eq. (7), this prediction is smaller than the estimate of the branching ratio from CLEO data in Eq. (5) by about a factor of 6.

The parameters  $K_{np}$  and  $p_0$  of the event-generator model can be adjusted so that the predictions of the model in Eqs. (6) and (7) agree with the CLEO results in Eqs. (4) and (5). Setting Eqs. (6) and (4) equal, we get  $K_{np}p_0^3 = (53 \pm 5 \text{ MeV})^3$ . Setting Eqs. (7) and (5) equal, we get the estimate  $p_0 \approx 140$  MeV. Allowing for a statistical error of  $\pm 1/\sqrt{3}$  in Eq. (5), the estimate for  $p_0$  ranges from 105 MeV to 163 MeV. Combining the two results, we obtain the estimate  $K_{np} \approx 0.05$  with an error that is at least  $\pm 0.03$ . The large errors in our estimates for  $p_0$  and  $K_{np}$  come from the small number of  $\overline{d} + d$  candidates observed in the experiment. It is somewhat surprising that  $K_{np}$  is one or two orders of magnitude smaller than 1. Pythia predicts that 3.6% of the  $\Upsilon \to ggg$  events include np and therefore also two antibaryons. In these events, almost half the 9.46 GeV of available energy goes into the rest energy of the four baryons and antibaryons. The predictions of an event generator for rare events like these can be expected to have large errors unless they are tuned to data. Since double baryon production was not used in the tuning of Pythia, it is plausible that there is a large error in its prediction for inclusive np production. If Pythia significantly overpredicts the probability of creating an np pair, the standard coalescence parameter  $p_0 = 80$  MeV must also underpredict the probability of their binding to form d, at least in the process  $\Upsilon \to ggg$ .

#### IV. THE X(3872) PRODUCTION CONTROVERSY

Hadronic event generators have been used by two different groups to estimate the production rate of the X(3872). Their estimates differ by orders of magnitude and lead to opposite conclusions about whether the X(3872) can be a loosely-bound charm meson molecule. In this section, we present a critical evaluation of those estimates.

#### A. Estimates of the X(3872) production rate

The quantum numbers of the X(3872) have been narrowed down experimentally to two possibilities,  $1^{++}$  or  $2^{-+}$ , by the observation of its decay into  $J/\psi\gamma$  [23] and by an analysis of its decays into  $J/\psi\pi^+\pi^-$  [24]. The observation of its decay into  $D^0\bar{D}^0\pi^0$  [25], whose threshold is lower by only about 7 MeV, disfavors spin 2 because of angular momentum suppression. On the other hand, a recent analysis of decays into  $J/\psi\pi^+\pi^-\pi^0$  favors negative parity [26]. Thus whether the quantum numbers of the X(3872) are  $1^{++}$  or  $2^{-+}$  remains an open experimental question. We will assume that they are  $1^{++}$ , in which case the X(3872) must be a loosely-bound charm meson molecule whose particle content is

$$X = \frac{1}{\sqrt{2}} \left( D^{*0} \bar{D}^0 + D^0 \bar{D}^{*0} \right).$$
(8)

Thus, if the event-generator model can be used to calculate the production rate of loosely-bound hadronic moelcules, it should be applicable to the X(3872).

The production of X(3872) in high energy hadron collisions comes from two mechanisms: the production of b hadrons followed by their weak decay into X(3872) and the prompt production of X(3872) through QCD mechanisms. The prompt cross section for X(3872) at the Tevatron can be estimated from measurements by the CDF Collaboration [27]. The cross section for X(3872) with transverse momentum  $p_T > 5$  GeV and rapidity |y| < 0.6 is [15, 16]

$$\sigma[X(3872)] \operatorname{Br}[X \to J/\psi \pi^+ \pi^-] = 3.1 \pm 0.7 \text{ nb},$$
(9)

up to corrections for acceptances and efficiencies that are expected to be small. From measurements of decays of X(3872) produced in B meson decays, one can infer that the branching fraction for X(3872) to decay into  $J/\psi \pi^+\pi^-$  is less than about 10% [16]. Thus the experimental lower bound on the cross section for X(3872) is about 30 nb.

Two groups have used event generators to estimate the prompt cross section for the X(3872) at the Tevatron  $p\bar{p}$ collider [15, 16]. Both estimates are expressed in terms of naive cross sections for the inclusive production of  $D^{*0}\bar{D}^0$ and  $D^0\bar{D}^{*0}$  with relative momentum k integrated up to some maximum  $k_{\text{max}}$ . Hadronic event generators, such as Pythia or Herwig, can be used to calculate the naive cross sections for the charm meson pairs. These event generators are tuned to reproduce charm meson distributions in various high energy experiments, but they have not been tuned to reproduce charm meson pair distributions. Thus one should allow at least for an unknown normalizing factor  $K_{D^*\bar{D}}$ in their predictions for charm meson pair distributions.

The dramatic discrepancy between the estimates in Refs. [15, 16] does not depend on the event generators. In Ref. [15] (BGPPS), the authors proposed an upper bound on the prompt cross section for the X(3872):

$$\sigma[X(3872)] < \frac{1}{2} K_{D^*\bar{D}} \left( \sigma_{\text{naive}}[D^{*0}\bar{D}^0(k < k_{\text{max}})] + \sigma_{\text{naive}}[D^0\bar{D}^{*0}(k < k_{\text{max}})] \right).$$
(10)

Their prescription for  $k_{\text{max}}$  was proportional to the binding momentum  $\gamma_X = \sqrt{2\mu E_X}$  of the X(3872), where  $\mu$  is the reduced mass of  $D^{*0}\bar{D}^0$ . In Ref. [16] (AB), the authors proposed an order-of-magnitude estimate for the prompt cross section for the X(3872):

$$\sigma[X(3872)] \approx \frac{3\pi\gamma_X}{k_{\max}} K_{D^*\bar{D}} \left( \sigma_{\text{naive}}[D^{*0}\bar{D}^0(k < k_{\max})] + \sigma_{\text{naive}}[D^0\bar{D}^{*0}(k < k_{\max})] \right).$$
(11)

Their prescription for  $k_{\text{max}}$  was the inverse of the range of the interactions between the charm mesons, give or take a factor of 2. Taking  $1/m_{\pi}$  as an estimate of the range, their prescription reduced to  $k_{\text{max}} = m_{\pi}$ , give or take a factor of 2. Now the naive cross sections in Eqs. (10) and (11) scale like  $k_{\text{max}}^3$  from phase space. The ratio of the estimate in Eq. (11) with  $k_{\text{max}} = m_{\pi}$  to the proposed upper bound in Eq. (10) with  $k_{\text{max}} = \gamma_X$  is therefore  $6\pi(m_{\pi}/\gamma_X)^2$ . For  $E_X = 0.4$  MeV, this ratio is about 530. Thus the estimate in Eq. (11) is more than two orders of magnitude larger than the proposed upper bound in Eq. (10). This dramatic discrepancy implies that there must be a serious conceptual error in the derivation of either the upper bound in Eq. (10) or the estimate in Eq. (11) or both.

In Ref. [15], BGPPS used both Pythia and Herwig to calculate the upper bound in Eq. (10) for the prompt X(3872) cross section at the Tevatron. They used measurements of  $D^0D^{*-}$  production at the Tevatron to determine the normalizing factor  $K_{D^*\bar{D}}$ . The upper bounds on  $\sigma[X]$  calculated by BGPPS using  $k_{\text{max}} = 35$  MeV were 0.11 nb using Pythia and 0.07 nb using Herwig. These theoretical upper bounds are more than two orders of magnitude smaller than the experimental lower bound of about 30 nb implied by Eq. (9). BGPPS concluded that the X(3872) was unlikely to be a loosely-bound charm meson molecule.

This conclusion was challenged in Ref. [16]. AB pointed out that the constituents of a loosely-bound S-wave molecule need not be created with relative momentum of order the binding momentum  $\gamma_X$ . Rescattering of the constituents In Ref. [16], AB used Pythia to calculate the estimate in Eq. (11) for the prompt X(3872) cross section at the Tevatron. They also used Madgraph to generate the Monte Carlo events more efficiently. They followed Ref. [15] in using measurements of  $D^0 D^{*-}$  production at the Tevatron to determine the normalizing factor  $K_{D^*\bar{D}}$ . The required factor ranges from 0.7 to 1.6 depending on the specific data used to determine the normalization. For  $E_X = 0.3$  MeV and  $k_{\max} = m_{\pi}$ , they obtained the estimate  $\sigma[X] \approx 6$  nb. The experimental lower bound of about 30 nb implied by Eq. (9) can be accomodated by choosing  $k_{\max} > 300$  MeV. Given the large uncertainties, AB concluded that the observed prompt production rate of the X(3872) at the Tevatron is compatible with its identification as a loosely-bound charm meson molecule.

The dramatic difference in the conclusions of Refs. [15] and [16] concerning the nature of the X(3872) comes from the dramatic conflict between the upper bound in Eq. (10) and the estimate in Eq. (11). We proceed to reexamine the derivation of these results. For simplicity, we carry out the discussion in the specific context of the deuteron. This avoids the notational complexity associated with constituents of the X(3872) being the superposition of charm mesons given in Eq. (8).

#### B. Upper bound of Ref. [15] applied to the deuteron

We first consider the upper bound in Eq. (10), which was derived by BGPPS in Ref. [15]. The analogous upper bound for the inclusive production of the deuteron is

$$\sigma[d] < K_{np} \ \sigma_{\text{naive}}[np(k < k_{\text{max}})]. \tag{12}$$

The prescription of BGPPS for  $k_{\text{max}}$  will be described below. Their derivation of this upper bound begins by expressing the inclusive cross section as the square of the production amplitude, summed over additional particles in the final state. The production amplitude is approximated by the product of the momentum-space wavefunction  $\psi(k)$  for the deuteron and the production amplitude for an np pair with relative momentum k, integrated over the vector  $\mathbf{k}$ . The range of the integral over  $\mathbf{k}$  can be restricted to the region  $0 < k < k_{\text{max}}$  in which the integrand has significant support. By applying the Schwartz inequality to the square of the production amplitude, one can derive the inequality

$$\sigma[d] \le \sigma[np(k < k_{\max})] \int \frac{d^3k}{(2\pi)^3} |\psi(k)|^2 \ \theta(k < k_{\max}).$$
(13)

The last factor is the incomplete normalization integral for the wavefunction of the molecule, so it is less than 1. If the cross section  $\sigma$  for np with  $k < k_{\text{max}}$  is dominated by generic hadronic scattering processes, it can be approximated by a naive cross section  $\sigma_{\text{naive}}$  that is not informed about the binding mechanism for the molecule. It  $\sigma_{\text{naive}}$  is calculated using an event generator, one should also allow for a normalization factor  $K_{np}$  for the production of a pair of baryons. This gives the upper bound in Eq. (12).

While the derivation of the upper bound in Eq. (12) is plausible, its validity hinges on the value of  $k_{\text{max}}$ . The right side of Eq. (12) is a strictly increasing function of  $k_{\text{max}}$ , so the inequality is certainly satisfied for sufficiently large  $k_{\text{max}}$ . The issue is whether the prescription for  $k_{\text{max}}$  used by BGPPS is valid for a loosely-bound molecule. Their prescription was not stated clearly in Ref. [15], but a partial clarification is given in Ref. [28]. It can be expressed as  $k_{\text{max}} = k_0 + \Delta k$ , where  $k_0$  and  $\Delta k$  are the typical momentum and the momentum spread in the bound state. Their prescription for  $k_0$  seems to be the binding momentum:  $k_0 = \gamma_d \equiv \sqrt{m_N E_d}$ . Their prescription for  $\Delta k$  seems to be the minimum spread in the momentum that is allowed by the uncertainty principle for a wavefunction whose rms separation is  $\gamma_d^{-1}$ :  $\Delta k = \gamma_d/2$ . (The universal prediction for the rms separation in a loosely-bound molecule is  $\gamma_d^{-1}/\sqrt{2}$ .) Since both  $k_0$  and  $\Delta k$  are proportional to  $\gamma_d$ , we can summarize their prescription by  $k_{\text{max}} = 1.5 \gamma_d$ . We proceed to critically examine this prescription.

The prescription  $k_{\text{max}} = k_0 + \Delta k$  in Ref. [15] is completely arbitrary. One could equally well have used the prescription  $k_{\text{max}} = ak_0 + b\Delta k$ , where a and b are numerical coefficients that are not too much larger than 1. This is important, because the naive cross section in Eq. (12) scales like  $k_{\text{max}}^3$  and is therefore very sensitive to  $k_{\text{max}}$ . A factor of 2 change in  $k_{\text{max}}$  will change the upper bound by almost an order of magnitude.

The prescriptions for  $k_0$  and  $\Delta k$  used in Ref. [15], which are both proportional to  $\gamma_d$ , are not only arbitrary but they are physically incorrect. More natural choices would have been the mean momentum  $\bar{k}$  and the standard deviation

 $\Delta k$  for a loosely-bound molecule with binding momentum  $\gamma_d$ . The universal wavefunction in momentum space for such a molecule is

$$\psi(k) = \frac{\sqrt{\gamma_d}}{\pi (k^2 + \gamma_d^2)}.$$
(14)

With this wavefunction,  $\bar{k}$  is logarithmically ultraviolet divergent and  $\Delta k$  is linearly ultraviolet divergent. The ultraviolet divergences are cut off by the range of the interaction between the constituents. In the case of the deuteron, an appropriate choice for the range is the effective range  $r_t = 1.76$  fm for np scattering in the spin-triplet channel. The physical interpretation of the divergences is that  $\bar{k}$  is proportional to  $\gamma_d$ , with a coefficient that scales as  $\log(1/\gamma_d r_t)$ , and that  $\Delta k$  scales as  $1/r_t$ .

That the upper bound in Eq. (12) with the prescription  $k_{\text{max}} = 1.5 \ \gamma_d$  is not valid can also be demonstrated on phenomenological grounds. We can regard Eq. (1) with  $p_0 = 80 \text{ MeV}$  as an empirical deuteron cross section determined from the analysis in Ref. [22]. The binding momentum of the deuteron is  $\gamma_d = 46 \text{ MeV}$ , so 1.5  $\gamma_d \approx 70 \text{ MeV}$ . Since  $k_{\text{max}} = 70 \text{ MeV}$  is smaller than  $p_0 = 80 \text{ MeV}$ , the proposed upper bound is smaller than the empirical deuteron cross section. A more plausible choice for the upper limit  $k_{\text{max}}$  in Eq. (12) is  $1/r_t \approx 110 \text{ MeV}$ . If we set  $k_{\text{max}} = 110 \text{ MeV}$ , the upper bound is larger than the empirical deuteron cross section in Eq. (1) by about a factor of 2.6.

#### C. Estimate of Ref. [16] applied to the deuteron

We next consider the estimate in Eq. (11), which was derived by AB in Ref. [16]. The analogous order-of-magnitude estimate for the case of the deuteron is

$$\sigma[d] \approx \frac{3}{4} \left(\frac{3\pi\gamma_d}{k_{\max}}\right) K_{np} \ \sigma_{\text{naive}}[np(k < k_{\max})], \tag{15}$$

where  $k_{\text{max}} = 1/r_t$ , give or take a factor of 2. This estimate is based on a rigorous relation between the cross section for a loosely-bound S-wave molecule and the cross section for its constituents that follows from the Migdal-Watson theorem [29]. According to the Migdal-Watson theorem, the production amplitude for the constituents can be expressed as the product of their scattering amplitude  $(\gamma_d + ik)^{-1}$ , where  $\gamma_d$  is the binding momentum of the molecule, and a slowly varying function of the relative momentum k that depends on the short-distance details of the production process. The production amplitude for the molecule has the same short-distance factor. Eliminating the short-distance factor, we obtain a rigorous relation between the cross sections for the molecule and its constituents. In the case of the deuteron, the relevant np scattering channel is the  ${}^{3}S_{1}$  channel and the relation is

$$\frac{d\sigma}{dk}[np(^{3}S_{1},k)] = \frac{k^{2}}{\pi\gamma_{d}(k^{2}+\gamma_{d}^{2})}\sigma[d].$$
(16)

If we integrate over the relative momentum up to  $k_{\rm max}$ , the relation becomes

$$\sigma[d] = \frac{\pi \gamma_d}{k_{\max} - \gamma_d \arctan(k_{\max}/\gamma_d)} \sigma[np(^3S_1, k < k_{\max})].$$
(17)

This rigorous relation holds for any  $k_{\text{max}}$  in the region  $k_{\text{max}} \ll 1/r_t$ , where  $r_t$  is the S-wave effective range, up to corrections suppressed by  $k_{\text{max}}r_t$ . Eq. (17) implies that the cross section for d is equal to that for np if  $k_{\text{max}} = 4.5 \gamma_d$ :

$$\sigma[d] = \sigma[np({}^{3}S_{1}, k < 4.5 \ \gamma_{d})].$$
(18)

This relation does not apply to the deuteron, because the condition 4.5  $\gamma_d \ll 1/r_t$  is violated. However the analogous relation might apply to more weakly bound molecules, such as the X(3872).

If we take the limit  $\gamma_d \to 0$  in the rigorous relation in Eq. (17), we see that the deuteron cross section decreases to 0 as  $E_d^{1/2}$  as its binding energy decreases to 0. This agrees with the conventional wisdom that the cross section for a loosely-bound molecule should go to 0 as its binding energy goes to 0. However naive phase space considerations suggest that the cross section should decrease as  $E_d^{3/2}$ . For example, in the coalescence model, the order-of-magnitude of the coalescence parameter  $p_0$  is often estimated by assuming that it is proportional to the binding momentum  $\gamma_d$ , which would imply that the cross section decreases as  $E_d^{3/2}$ . The actual suppression factor  $E_d^{1/2}$  is much milder than the naive suppression factor  $E_d^{3/2}$ .

In Ref. [16], AB used the rigorous relation in Eq. (17) to obtain an order-of-magnitude estimate of the cross section for a loosely-bound molecule. They chose  $k_{\text{max}}$  to be the scale of the relative momentum k at which the universal

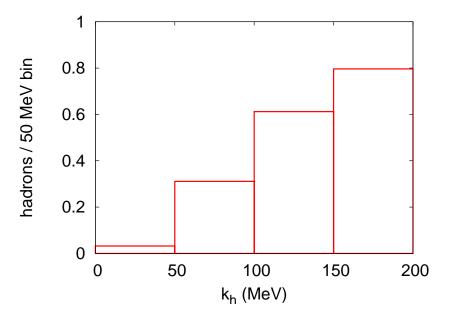


FIG. 3: Average number of hadrons in  $\Upsilon \to ggg \to \bar{n}\bar{p}(k_1 < 80 \text{ MeV}) + X$  events generated by Pythia with respect to  $k_h$ , the smaller of the relative momenta of the hadron h with respect to  $\bar{n}$  and  $\bar{p}$ .

differential cross section  $d\sigma/dk$ , which approaches  $\sigma[d]/\pi\gamma_d$  at large k, becomes comparable to the naive differential cross section, which scales as  $k^2$  for small k. The resulting estimate for  $\sigma[d]$  is given in Eq. (15). The factor of 3/4 accounts for 3 of the 4 spin states of np being in the spin-triplet channel in which there is binding. Since the naive cross section in Eq. (15) scales like  $k_{\text{max}}^3$ , the estimate for  $\sigma[d]$  is proportional to  $k_{\text{max}}^2$ . An estimate of the momentum  $k_{\text{max}}$  at which  $d\sigma/dk$  becomes comparable to the  $d\sigma_{\text{naive}}/dk$  is required to complete the estimate of  $\sigma[d]$ .

As an estimate of  $k_{\text{max}}$ , AB proposed the reciprocal of the effective range, give or take a factor of two. In the case of the deuteron, the central estimate would be  $1/r_t \approx 110$  MeV. Comparing with the phenomenological estimate in Eq. (1), we see that this would correspond to a coalescence parameter  $p_0 = (9\pi\gamma_d/4r_t^2)^{1/3} \approx 160$  MeV. Varying  $k_{\text{max}}$  by a factor 2, this theoretical estimate of the coalescence parameter  $p_0$  varies from 100 MeV to 250 MeV. This estimate is larger than the standard value 80 MeV obtained in Ref. [22]. It is interesting to note that the estimate of  $p_0$  obtained from data on  $\Upsilon$  decays in Section III B is also larger than the standard value.

#### D. Hadronic activity

In Ref. [20], the authors raised an issue concerning hadronic activity near a loosely-bound molecule. If additional hadrons are produced that have small momentum relative to the molecule, their interactions with the constituents of the molecule can complicate the production process. The order-of-magnitude estimate in Eq. (15), which was based on the Migdal-Watson theorem, did not take into account the possibility of additional hadrons with small relative momentum. The authors suggested that this cast doubts on the applicability of the Migdal-Watson theorem to an estimate of the production rate in cases where there is significant hadronic activity near the molecule.

In the case of anti-deuteron production in  $\Upsilon$  decays, the only experimental information on the hadronic activity is that in the single  $\bar{d} + d$  candidate event that was displayed in Ref. [9], the  $\bar{d}$  and d were accompanied by 6 charged pions. One can use an event generator to predict the hadronic activity. In Fig. 3, we show the prediction of Pythia for the number of additional hadrons h produced in the events  $\Upsilon \to ggg \to \bar{n}\bar{p}(k_1 < p_0) + X$  as a function of the smaller of the relative momenta of the hadron h with respect to  $\bar{n}$  and  $\bar{p}$ , which we denote by  $k_h$ . The average number of additional hadrons with  $k_h < 100$  MeV is about 0.3. More than 60% of the events have no such additional hadron. Thus hadronic activity near the anti-deuteron does not seem to be a serious complication in  $\Upsilon \to ggg$ .

In the case of the production of the X(3872) at the Tevatron, the hadronic activity is larger because the Tevatron is a high-energy hadron collider. In Ref. [20], event generators were used to predict the hadronic activity near a pair of charm mesons with small relative momentum. They found that in events that include a charm-meson pair with k < 300 MeV, there are typically two or three additional hadrons whose relative momentum with respect to one of the charm mesons satisfies  $k_h < 100$  MeV. Less than 10% of the events have no such additional hadrons. Since the estimate in Eq. (15) can accommodate the experimental lower bound on the prompt cross section for X(3872) only if  $k_{\text{max}} > 300$  MeV, this level of hadronic activity is significant.

However hadronic activity near the molecule does not necessarily invalidate the use of the Migdal-Watson theorem. The interaction between a generic low-momentum hadron and a constituent of a loosely-bound S-wave molecule is much weaker than the interaction between the two constituents. For relative momentum k in the range  $\gamma_X < k < m_{\pi}$ , the interaction between the constituents is so strong that it saturates the unitarity bound. For generic hadrons, the interaction strength may be close to the unitarity bound for  $k \sim m_{\pi}$ , but it does not increase at lower k. An exception is a pion and D meson with relative momentum of about 40 MeV, which have a P-wave resonance through the  $D^*$ . With this exception, it is plausible that the effects of low-momentum hadrons can be treated as perturbations to the interactions between the constituents of the molecule.

#### V. DISCUSSION

The deuteron and the X(3872) (provided its quantum numbers are  $J^{PC} = 1^{++}$ ) are manifestations of looselybound S-wave hadronic molecules. As such, they have universal properties that are completely determined by their binding energies. There have been several attempts in the literature to calculate their production rates based on the predictions of hadronic event generators for the production rates of their constituents. In the coalescence model, the production rate of the molecule is the production rate of a pair of its constituents integrated over the relative momentum up to  $p_0$ , as in Eq. (1). In the event-generator model defined in Section II, the production rate for the pair of constituents is also multiplied by a normalizing factor K, as in Eq. (2). It should be emphasized that these are purely phenomenological models. The closest thing to a rigorous justification is the relation between the cross section for a loosely-bound S-wave molecule and the integrated cross section for its constituents in Eq. (17).

In the spirit of hadronic event generators, the coalescence parameter  $p_0$  and the normalizing factor K should be treated as phenomenological parameters to be determined by experiment. Theoretical estimates of these parameters, such as Eq. (15) with  $k_{\text{max}} = 1/r_t$ , can only provide order-of-magnitude estimates. Quantitative predictions using the event-generator model require the determination of  $p_0$  and K from data. The normalizing factor K is necessary, because data on pairs of constituents are generally not among the inputs used to tune the event generator. Since the naive cross section is proportional to  $p_0^3$ , the inclusive cross section for production of a molecule is sensitive only to  $Kp_0^3$ . One way to determine K is from separate measurements of the production rate of a pair of constituents. For example, in Refs. [15, 16], the cross section for  $D^0D^{*-}$  was used to determine the normalizing factor  $K_{D^*\bar{D}}$  for the X(3872). Another way to determine K is from separate measurements of both the molecule and the molecule plus its antiparticle. For example, CLEO data on inclusive  $\bar{d}$  and inclusive  $\bar{d} + d$  was used in Section III to estimate the normalizing factor  $K_{np}$  for the deuteron.

We applied these considerations to the production of the anti-deuteron in  $\Upsilon$  decays, confronting the predictions of the event-generator model with measurements by the CLEO Collaboration. The measurement of the direct branching fraction for inclusive  $\bar{d}$  in Eq. (4) determines the combination  $K_{np}p_0^3$ . The estimate of the branching ratio for inclusive  $\bar{d}+d$  and inclusive  $\bar{d}$  in Eq. (5) can then be used to obtain separate estimates for  $K_{np}$  and  $p_0^3$ . These estimates suggest that the inclusive production rate for  $\bar{n}\bar{p}$  is overestimated by Pythia, perhaps by an order of magnitude, and that the standard coalescence parameter  $p_0$  underpredicts the probability for formation of a  $\bar{d}$  from  $\bar{n}$  and  $\bar{p}$  with small relative momentum.

We discussed the proposed upper bound on the production rate of a loosely-bound S-wave molecule that was derived in Ref. [15]. If applied to the prompt cross section for the X(3872) at the Tevatron, the upper bound is more than two orders of magnitude smaller than the observed cross section, leading the authors of Ref. [15] to conclude that the X(3872) can not be a loosely-bound molecule. The analogous upper bound for the deuteron is given by Eq. (12) with  $k_{\text{max}} = k_0 + \Delta k$ , where  $k_0 = \gamma_d$  and  $\Delta k = \gamma_d/2$  are estimates of the typical momentum and the momentum spread in the bound state. We demonstrated that the upper bound with this prescription for  $k_{\rm max}$  is invalid both on phenomenological and theoretical grounds. The phenomenological grounds are that the prescription  $k_{\rm max} = 1.5 \ \gamma_d \approx 70 \ {\rm MeV}$  is smaller than the standard coalescence parameter  $p_0 = 80 \ {\rm MeV}$ . This indicates that the anti-deuteron cross sections used to determine  $p_0$  must exceed the proposed upper bound. The prescription for  $k_{\rm max}$  in Ref. [15] is not only arbitrary, but it is based on the inappropriate use of the minimal uncertainty principle for a Gaussian wavefunction to estimate  $\Delta k$ . A weakly-bound S-wave molecule maximizes the uncertainty, because  $\langle k^2 \rangle = \infty$ . Thus the prescription in Ref. [15] underestimates the value of  $k_{\text{max}}$  required for Eq. (12) to be an upper bound on the cross section. Since the naive np cross section scales like  $k_{\max}^3$ , the upper bound on  $\sigma[d]$  is underestimated by a much larger factor. Similarly, the upper bound on the prompt cross section for the X(3872) at the Tevatron is underestimated by more than an order of magnitude. We conclude that there is no clear conflict between the observed cross section for X(3872) and the interpretation of the X(3872) as a loosely-bound charm-meson molecule.

The event-generator model should give the most accurate predictions for experiments that are the most similar

to the ones used to determine the parameters K and  $p_0$ . Predictions for the LHC using parameters determined at the Tevatron should be particularly accurate. For the antideuteron, the inclusive differential cross section  $d\sigma/dy$  at central rapidity y = 0 has been measured by the E735 collaboration [10]. This measurement can be used to determine  $K_{np}p_0^3$ , which can then be used to predict cross sections for anti-deuteron production at the LHC. For the X(3872), the prompt cross section in Eq. (9), which was obtained from CDF measurements at the Tevatron, can be used to determine  $K_{D^*\bar{D}} p_0^3 \operatorname{Br}[X \to J/\psi \pi^+\pi^-]$ . This combination can then be used to predict the prompt production rate of  $X \to J/\psi \pi^+\pi^-$  at the LHC.

One of the drawbacks of the event-generator model is the enormous number of events that must be generated to get reasonable statistics on the production rate of a pair of constituents with small relative momenta. In the case of the X(3872), there is a more efficient way to calculate the production rate. The production of a charm meson pair with small relative momentum requires the creation of a  $c\bar{c}$  pair with small relative momentum. In the NRQCD factorization formalism, the production of the charm meson pair can be expressed as the sum of products of parton cross sections for the creation of the  $c\bar{c}$  pair and NRQCD matrix elements for the formation of the charm mesons [30]. At leading order in  $\alpha_s$ , three of the four S-wave color/spin  $c\bar{c}$  channels have cross sections that are suppressed at large transverse momentum  $p_T$  by at least a factor of  $m_c^2/p_T^2$ . The  $c\bar{c}$  channel that is not suppressed at leading order in  $\alpha_s$  is color-octet  ${}^{3}S_{1}$ . Thus the simplest NRQCD factorization formula that can approximate the predictions of the event-generator model is to keep only the color-octet  ${}^{3}S_{1}$  term in the differential cross section:

$$d\sigma[X(3872)] = d\hat{\sigma}[c\bar{c}_8(^3S_1)] \langle \mathcal{O}_8^X(^3S_1) \rangle.$$

$$\tag{19}$$

The multiplicative constant  $\langle \mathcal{O}_8^X({}^3S_1) \rangle$  plays the same role as  $K_{D^*\bar{D}}p_0^3$  in the event-generator model. In Ref. [16], the combination  $\langle \mathcal{O}_8^X({}^3S_1) \rangle$  Br $[X \to J/\psi \pi^+\pi^-]$  was determined from the prompt cross section at the Tevatron in Eq. (9) and then used to predict the differential cross section of  $X \to J/\psi \pi^+\pi^-$  in various experiments at the LHC. Similar results could presumably be obtained using the event-generator model, but the enormous number of Monte Carlo events that would have to be generated makes it impractical. The NRQCD factorization approach is much more efficient, because the parton differential cross section  $d\hat{\sigma}[c\bar{c}_8({}^3S_1)]$  at leading order in  $\alpha_s$  is known analytically.

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