

Non-Markovian dynamics of bottomonia in the QGP

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The evolution of quarkonia in the QGP medium can be described through the formalism of open quantum systems (OQS). In previous works with OQS, the quarkonium evolution was studied by working in either quantum Brownian or optical regime. In this paper, we set up a general non-Markovian master equation to describe the evolution of the quarkonia in the medium. Because of the non-Markovian nature, it cannot be cast in Lindblad form, which makes it challenging to solve. We numerically solve the master equation for $\Upsilon(1S)$ without considering stochastic jumps for Bjorken and viscous hydrodynamic background at energies relevant to the large hadron collider (LHC) and relativistic heavy ion collider (RHIC). We quantify the effect of the hierarchy between the system timescale, $\tau_S \sim 1/E_b$, and the environment timescale, τ_E , on quarkonium evolution and show that it significantly affects the nuclear modification factor. A comparison of our results with the existing experimental data from the LHC and RHIC is presented.

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I. INTRODUCTION

The key processes governing the dynamics of quarkonia (bound states of a heavy quark Q and its antiquark $\bar{Q}$) in the quark-gluon plasma (QGP) have been recognized for a long time. They include gluodissociation [1,2], screening of the interaction between Q and $\bar{Q}$ [3], and dissociation through t -channel scattering with medium [4–6]. They have been widely used to address the phenomenology of quarkonia at RHIC and LHC (see Refs. [11,12] for reviews).

Additional insight into these processes has been obtained by studying them in an effective field theory (EFT) for quarkonium states: potential nonrelativistic QCD (pNRQCD) [13]. pNRQCD relies on the hierarchy between the energy scales $M \gg 1/r \gg E_b$, where M is the mass of Q , $1/r$ is the inverse of the relative separation between $Q - \bar{Q}$, and E_b is the binding energy of quarkonia. It is a theory of singlet $[S(\mathbf{r}, t)]$ and octet $[\mathcal{O}(\mathbf{r}, t)]$ wave functions that describe the $Q - \bar{Q}$ state, and gluonic and light quark modes with momenta and energies $\lesssim E_b$. The Lagrangian up to order $E_b^2 r$ has the form

$$\begin{aligned} L_{\text{pNRQCD}} = \int d^3\mathbf{r} \text{tr} & \left(S(\mathbf{r}, t)^\dagger [i\partial_0 - h_s] S(\mathbf{r}, t) \right. \\ & + \mathcal{O}(\mathbf{r}, t)^\dagger [iD_0 - h_o] \mathcal{O}(\mathbf{r}, t) \\ & + gV_A(r) [\mathcal{O}^\dagger(\mathbf{r}, t) \mathbf{r} \cdot \mathbf{E} S(\mathbf{r}, t) \\ & + S^\dagger(\mathbf{r}, t) \mathbf{r} \cdot \mathbf{E} \mathcal{O}(\mathbf{r}, t)] \\ & \left. + \frac{V_B(r)}{4} \{ \mathcal{O}^\dagger(\mathbf{r}, t), \{ \mathbf{r} \cdot g\mathbf{E}, \mathcal{O}(\mathbf{r}, t) \} \} \right) + L_{\text{light}}. \end{aligned} \quad (1)$$

Here, $h_s = p^2/M + v_s$ ($h_o = p^2/M + v_o$) is the singlet (octet) Hamiltonian, and $\mathbf{E}$ is the chromoelectric field. $v_{s,o}$ [similarly $V_{A,B}(r)$] are Wilson coefficients (which can depend on $\mathbf{r}$ and ∂_r) that are determined by dynamics occurring at energy scales above E_b .

In the thermal medium, additional scales—for example, the temperature T and the (longitudinal) gluonic screening mass m_D —play a role. They can modify $v_{s,o}$ [14]. The EFT can be analyzed assuming different hierarchies between the intrinsic scales of the $Q - \bar{Q}$ state, $1/r$, E_b , and the thermal scales, and it has been shown that the relative importance of the different processes depends on these hierarchies [14–17]. For bottomonia, $M \gg 1/r \gg T$, but the hierarchy between T and E_b depends on the bottomonium state and can change as the QGP cools [18].

The power of the EFT approach is that it allows us to separate the dynamics of the $Q - \bar{Q}$ state from the dynamics of the modes at scales $\gtrsim E_b$. The latter can then be modeled (one can study the systematic dependence of the results on the parameters in the usual manner by varying

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the parameters of the models within physically motivated regions), calculated using weak-coupling techniques at high temperatures or calculated nonperturbatively using lattice QCD (see Ref. [19] for reviews).

Examples already mentioned above are $v_{s,o}$. These “potentials” are known to three-loop order in QCD [20–23]. They have also been calculated on the lattice in a thermal medium [24–28]. $V_{A,B}(r) = 1$ at leading order [29].

Another illustrative example is the decay width of a state $|\psi\rangle$ in the thermal medium. This has the form [14]

$$\frac{1}{\tau_\psi} = \frac{g^2}{3N_c} \sum_f |\langle f|\mathbf{r}|\psi\rangle|^2 f(k^0) \int \frac{d^3\mathbf{k}}{(2\pi)^3} \rho_{\text{EE}}(k^0, \mathbf{k})|_{k^0=\epsilon_f-\epsilon_\psi}, \quad (2)$$

where $f(k^0)$ is the Bose distribution and ρ_{EE} is a chromoelectric spectral function in the medium. Matrix elements like $\langle f|\mathbf{r}|\psi\rangle$ can be computed within the EFT [Eq. (1)]. On the other hand, the spectral function is a property of the thermal medium. It is proportional to the real part of the Fourier transform of a gauge-invariant chromoelectric field correlator [Eq. (12)]. One can estimate the correlator using weak coupling techniques [14,30–32], constrain it using the measurement of quarkonium spectral functions on the lattice [33–35], or calculate it [36,37] for strongly coupled supersymmetric theories sharing features with QCD using AdS/CFT techniques (see Ref. [38] for a review). Ideally, one would like to compute it nonperturbatively using lattice QCD techniques, though it is a challenging calculation because it is a real-time correlation function [39,40].

The Wilson coefficients of the EFT and the correlators of the chromoelectric field complete the microscopic input required to describe the dynamics of $Q - \bar{Q}$ in a static medium. Going from the microscopic theory to the phenomenology of quarkonia at LHC and RHIC requires two additional technical pieces:

- (1) The background medium evolves hydrodynamically after quickly reaching local thermal equilibrium (see Refs. [41–47] for reviews). Assuming local thermal equilibrium, the temperature in the neighborhood of the $Q - \bar{Q}$ state determines the dynamics of the state. In this paper, we use the results from the hydrodynamic model described in Ref. [48], which describes several aspects of the phenomenology of low-energy hadrons observed in heavy-ion collisions at the RHIC [49] and at the LHC [48,49] very well.
- (2) For temperatures encountered by the $Q - \bar{Q}$ in the QGP (few 100 MeV), the width of the states is not much smaller [18] than the binding energy. Furthermore, the timescale on which the medium evolves is $\sim \text{fm}$, again comparable to the inverse of the binding energy. Hence, one needs to follow

the quantum evolution of the $Q - \bar{Q}$ state [50–52]. Quantum systems (S) in contact with an external environment (E) are described using the open quantum systems (OQS) framework [53], in which master equations for the evolution equations for the $Q - \bar{Q}$ density matrix (ρ_S) are derived. We use this framework in this paper. (See Refs. [54–56] for reviews of applications OQS approaches to quarkonia.)

Previously, several works have derived and solved master equations for the evolution of ρ_S under various assumptions and approximations, and we will briefly review some of their key features to set the context for our calculation. The most convenient choice of the basis for describing the quantum system depends on the hierarchy between the intrinsic timescale ($\tau_S \sim 1/E_b$) and the system relaxation time [$\tau_R \sim \tau_\psi$ (Eq. (2))].

For $\tau_R \gg \tau_S$, the widths of the bound states are small compared to the splitting between them, and the energy eigenfunctions of the system Hamiltonian form a convenient basis. This is known as the quantum optical regime [53,54] and was studied in Refs. [57,58]. Furthermore, if we assume that the timescale for relaxation of the excitations in the environment τ_E is shorter than τ_R , by expanding the master equations second order in τ_E/τ_R [next-to-leading order (NLO)] one can write the master equations in a Lindblad [59,60] form. This Lindblad equation in the optical regime was derived and solved by converting it to coupled Boltzmann equations in Refs. [55,61–63].

If τ_R is not much less than τ_S , a more convenient basis is a basis of a continuum of states, for example, wave functions in position space. Furthermore, if we assume τ_E is shorter than τ_S , then by expanding the master equations at leading order (LO) or at NLO in τ_E/τ_S , one can write the master equations in a Lindblad form (quantum-Brownian regime). The Lindblad equations were derived in the weak-coupling approximation in Ref. [64] (LO) and Ref. [65] (NLO) and solved in Refs. [66,67]. Lindblad equations in the quantum-Brownian regime were also derived in the weak coupling approximation by a different group in Refs. [68–71] and solved by making semiclassical approximations [68–73] and numerically [74]. Using pNRQCD, Lindblad equations for $Q - \bar{Q}$ were derived in the quantum-Brownian regime and solved numerically in Refs. [75–78] (LO) and Refs. [34,35,79] (NLO).

The starting point for all these analyses is an operator equation for the time derivative of ρ_S of the form [80,81] described below in Eq. (8), which we show here for convenience,

$$\frac{\partial \rho_S(t)}{\partial t} = - \sum_{m,n} \int_0^t ds \Gamma_{mn}(t-s) [\mathbf{V}_S^m(t), \mathbf{V}_S^n(s) \rho_S(t)] + \text{H.c.}, \quad (3)$$

where $\Gamma_{mn}(t-s)$ are environmental correlation functions (in our case chromoelectric correlators) which decay on timescales $t-s \sim \tau_E$.

If this timescale is short compared to the timescale of the variation of $\mathbf{V}_S^n(s)$ (τ_S) and the observation time (t), then the time evolution of ρ_S can be written as a Lindblad equation [59,60]. (See Appendix A for a brief review of the derivation.) Physically, if $\tau_E \ll \tau_S$, any memory of the S-E exchanges is quickly lost, and the S evolution is Markovian. Evolution in this regime is sensitive only to the zero-frequency limit of the environment correlators, $\lim_{\omega \rightarrow 0} \tilde{\Gamma}_{mn}(\omega)$ [we will refer to the Fourier transform of $\Gamma_{mn}(t)$ as $\tilde{\Gamma}_{mn}(\omega)$].

However, for bottomonia in the QGP, $1/\tau_S \sim$ few 100 MeV is comparable to $1/\tau_E \sim T$, which also has the magnitude of a few 100 MeV [18]. Thus, it is necessary to solve the $Q - \bar{Q}$ master equations for $\tau_E \sim \tau_S$, using the master equation with memory [Eq. (3)]. In particular, this can be important for $\Upsilon(1S)$, whose binding energy is the largest. The need for solving non-Markovian master equations in strongly coupled theories has also been recently emphasized in Ref. [37].

This is the main goal of this paper. The main technical advance in the paper is the numerical solution of the non-Markovian master equation using the method of stochastic unraveling [82] (see Sec. III for details) and calculating the survival probability for the $\Upsilon(1S)$ state. To our knowledge, this is the first calculation of the suppression of Υ states using a master equation with memory.

Thinking about Eq. (3) in Fourier space, the evolution of ρ_S is sensitive to $\tilde{\Gamma}_{mn}(\omega)$ up to frequencies $\omega \sim 1/\tau_E$. It has previously been shown that keeping the dependence of the chromoelectric correlator on ω in the calculation of the decay rate [Eq. (2)] leads to a substantial reduction of the decay rate [18,83] when compared to a calculation that approximates the correlator with its zero-frequency limit. In this paper, we show that in the OQS framework using the non-Markovian master equation also leads to a much smaller suppression than a LO calculation with otherwise identical system and medium parameters. We also show that the NLO Markovian equation [34,79] captures this important effect and gives results comparable to those obtained from the full master equation for most of the evolution (unless τ_E is larger than $1/T$), except for $T \lesssim 250$ MeV. The master equation is better controlled than the NLO Markovian equation at these lower temperatures.

Using medium and system parameters that describe the phenomenology of bottomonia at LHC [84–90] using NLO Markovian equations [34], we present results for the R_{AA} of $\Upsilon(1S)$ in 200 GeV Au-Au collisions at the RHIC and 2.76 and 5.02 TeV Pb-Pb collisions at the LHC. For $\tau_E \sim 1/T$, our calculation gives results for R_{AA} comparable in magnitude to that of NLO Markovian equations and gives results broadly in agreement with the suppression of $\Upsilon(1S)$

states obtained at LHC and underpredicts [91] the suppression at the RHIC [92]. We analyze the systematic dependence of the survival probability on τ_E .

However, addressing the phenomenology of quarkonia in heavy-ion collisions is not the central goal of this paper. There are some effects that have not been included in our calculations that might be important for that purpose. We list a few below:

- (1) Gluodissociation is an effect that has not been included beyond the static limit in master equations so far (see Ref. [55,61–63] for a semiclassical implementation, and see Ref. [67] for incorporation of gluodissociation in the stochastic Schrödinger equation) and may play an important role at lower temperatures.
- (2) Cold nuclear matter effects on the parton density functions might affect [93–97] the initial hard production of bottomonia in heavy ion collisions.
- (3) As we have not (yet) calculated the survival probability of the excited states, we cannot calculate the contribution to R_{AA} from their feed-down here.

A systematic analysis of the phenomenology will require including these effects and then refitting the medium transport coefficients (in particular the zero-frequency limit of the chromoelectric correlator, as it is not yet known independently). We leave this detailed program for the future and restrict ourselves to understanding the systematic effect of considering different hierarchies between τ_E and τ_S in this paper.

The plan of the paper is as follows. In Sec. II, we review the formalism and derive the master equations. In Sec. III, we discuss the algorithm and the numerical setup used for solving the master equations.

In Sec. IV, we describe our results. To get a clearer understanding, we first analyze the effect of memory in a time-independent medium in Sec. IV A. Effects in a simple Bjorken flow are analyzed in Sec. IV B. Results for realistic hydrodynamic backgrounds, with the closest connection to phenomenology at the RHIC and LHC, are shown in Sec. IV C.

Some technical details have been moved to the Appendix. In Appendix A, we briefly review the derivation of the LO Markovian equation. In Appendix B, we explore how memory effects change with T in a time-independent medium. In Appendix C, we motivate the choice of the form of the time-dependent correlator. Results for PbPb collisions at 2.76 TeV are given in Appendix D.

II. FORMALISM

In this section, we review the derivation of the general master equation for quarkonium dynamics.

Consider a system (S) interacting with the environment (E). The combined system and environment are isolated, so the density matrix of the total system evolves as

$$\frac{\partial \rho_{\text{tot}}(t)}{\partial t} = -i[H_{\text{tot}}, \rho_{\text{tot}}], \quad H_{\text{tot}} = H_S + H_E + H_I, \quad (4)$$

where H_S and H_E are the system and environment Hamiltonians, respectively. S and E interact through an interaction term H_I . The reduced density matrix of the system is calculated by tracing out the environment variables,

$$\rho_S = \text{Tr}_S[\rho_{\text{tot}}]. \quad (5)$$

In the interaction picture (denoted with a superscript I on the density matrix), taking H_I as the interaction, the evolution equation of ρ_S can be written as

$$\frac{\partial \rho_S^I(t)}{\partial t} = - \int_0^t ds \text{Tr}_E([H_I(t), [H_I(s), \rho_{\text{tot}}^I(s)]]). \quad (6)$$

At the initial time, S and E are typically not entangled (often the system starts in a pure state, as we assume here). Therefore, $\rho_{\text{tot}}(0) = \rho_S(0) \otimes \rho_E$. Since E is much larger than S, its density matrix does not change substantially during evolution [98] although S becomes entangled with E. If H_I is weak, however, $\rho_{\text{tot}}(s)$ can be approximated by $\rho_S(s) \otimes \rho_E$. This is known as the Born approximation [82]. Furthermore, if $H_I^2 \tau_E$ is much smaller than the inverse of the timescale on which ρ_S^I changes, then $\rho_S^I(s)$ in the s integrand can be replaced by $\rho_S^I(t)$ [82]. Corrections to these approximations go as H_I^4 and are small if $\tau_R \gg \tau_E$ since τ_R scales as H_I^2 . For quarkonia, this hierarchy follows from the multipole expansion as long as $1/r \gg T$.

With these approximations, Eq. (6) gives a master equation of the form

$$\frac{\partial \rho_S^I(t)}{\partial t} = - \int_0^t ds \text{Tr}_E([H_I(t), [H_I(s), \rho_S^I(t) \otimes \rho_E]]). \quad (7)$$

It is known in the literature as the Redfield equation [80,81]. Although the r.h.s. of Eq. (7) depends only on ρ_S at the instant t , Eq. (7) is not a Markovian equation since the operator $\text{Tr}_E(H_I(t)H_I(s)\rho_E)$ depends on times s between 0 and t .

H_I can be written as the sum of tensor products of E and S operators, $H_I = \sum_n \mathbf{E}_E^n \otimes \mathbf{V}_S^n$. After taking the trace over E, Eq. (7) can be rewritten as

$$\begin{aligned} \frac{\partial \rho_S^I(t)}{\partial t} = & - \sum_{m,n} \int_0^t ds \Gamma_{mn}(t,s) (\mathbf{V}_S^m(t) \mathbf{V}_S^n(s) \rho_S^I(t) \\ & - \mathbf{V}_S^n(s) \rho_S^I(t) \mathbf{V}_S^m(t)) + \text{H.c.}, \end{aligned} \quad (8)$$

where $\Gamma_{mn}(t,s) = \langle \mathbf{E}_E^m(t) \mathbf{E}_E^n(s) \rangle_E$ and only depends on $t-s$ for a static medium.

To find the specific form of Γ_{mn} and $\mathbf{V}_S^n$ for quarkonia, we use the pNRQCD Lagrangian [Eq. (1)]. In the center of

mass (CM) of the quarkonium state, the system Hilbert space features the singlet states $|s\rangle$ (the separation $\mathbf{r}$ is suppressed for clarity) and octet states $|a\rangle$ ($a = 1, \dots, 8$):

$$\begin{aligned} H_S &= h_s |s\rangle \langle s| + h_o |a\rangle \langle a| \\ H_I &= -g \mathbf{E}^a \cdot \mathbf{r} \left(\frac{1}{\sqrt{2N_c}} |s\rangle \langle a| + \frac{1}{\sqrt{2N_c}} |a\rangle \langle s| + \frac{d_{abc}}{2} |b\rangle \langle c| \right). \end{aligned} \quad (9)$$

The color structure of ρ_S can be further simplified by reducing it to blocks of singlet and octet components. The singlet and octet reduced density matrices are defined as $\rho_s = \langle s | \rho_S | s \rangle$ and $\rho_o = \sum_a \langle a | \rho_S | a \rangle$. Going back to the Schrödinger picture and changing the integration variable from s to $t-s$, the evolution equation for ρ_S [Eq. (8)] can be written as

$$\begin{aligned} \frac{\partial \rho_S(t)}{\partial t} &= -i(H_{\text{eff}} \rho_S(t) - \rho_S(t) H_{\text{eff}}^\dagger) \\ &+ \int_0^t ds \left(\sum_{n=1}^3 \Gamma_n(t, t-s) \mathbf{V}_n(-s) \rho_S(t) \mathbf{V}_n^\dagger(0) + \text{H.c.} \right), \\ H_{\text{eff}} &= H_S - i \int_0^t ds \sum_{n=1}^3 \Gamma_n(t, t-s) \mathbf{V}_n^\dagger(0) \mathbf{V}_n(-s). \end{aligned} \quad (10)$$

where $\{\mathbf{V}_n(t)\}$ [Eq. (10)] are time-dependent operators, and the index n labels their structure in color space: $n=1$ corresponds to $s \rightarrow o$, $n=2$ to $o \rightarrow s$, and $n=3$ to $o \rightarrow o$ transitions. The explicit form of $\mathbf{V}_n$ in s, o space is as follows:

$$\mathbf{V}_n(t) = \begin{cases} e^{ih_o t} \mathbf{r} e^{-ih_s t} & \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & n=1 \\ e^{ih_s t} \mathbf{r} e^{-ih_o t} \sqrt{\frac{1}{(N_c^2-1)}} & \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} & n=2 \\ e^{ih_o t} \mathbf{r} e^{-ih_o t} \sqrt{\frac{N_c^2-4}{2(N_c^2-1)}} & \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} & n=3. \end{cases} \quad (11)$$

The spatial indices of $\mathbf{V}_n$ are summed in Eq. (10).

The medium response functions Γ_n are obtained by tracing out the environment chromoelectric fields $\mathbf{E}$. For $n=1$, we have

$$\Gamma_1(t, t') = \frac{g^2}{6N_c} \text{Tr}_E(\mathbf{E}^a(t, \vec{0}) \mathcal{W}_{ab}(t, t') \mathbf{E}^b(t', \vec{0}) \rho_E), \quad (12)$$

where $\mathcal{W}_{ab}(t, t')$ is the adjoint Wilson line [35] joining $(t', \vec{0})$ and $(t, \vec{0})$. The correlators Γ_2 and Γ_3 have $\mathcal{W}$ at the ends (see Ref. [99] for a derivation of the correlators).

The insertion of $\mathcal{W}_{ab}$ makes Γ_n Gauge invariant. Since our results do not require $\Gamma_{2,3}$, for a simpler notation, we drop the subscript n and identify Γ with Γ_1 .

The operators $\mathbf{V}_n(t)$ evolve on the system timescale $\tau_S \sim 1/E_b$. The correlator $\Gamma(t)$ is significant when $t \lesssim \tau_E \sim 1/T$. In the quantum Brownian approximation, one assumes the hierarchy $\tau_E \ll \tau_S$. The operators $\mathbf{V}_n(t)$ can therefore be expanded as

$$\mathbf{V}_n(t) \sim e^{ih_\alpha t} \mathbf{r} e^{-ih_\beta t} \approx \mathbf{r} + it(h_\alpha \mathbf{r} - \mathbf{r} h_\beta) + \mathcal{O}\left[\left(\frac{\tau_E}{\tau_S}\right)^2\right], \quad (13)$$

where $\{\alpha = o, \beta = s\}$ for $n = 1$, $\{\alpha = s, \beta = o\}$ for $n = 2$, and $\{\alpha = o, \beta = o\}$ for $n = 3$.

As reviewed in the Introduction, truncating the expansion in Eq. (13) at the first term gives the LO [77] Lindblad equation, and keeping the term proportional to t gives the NLO [79] Lindblad equation. These Lindblad equations feature two real transport coefficients κ and γ defined as

$$\tilde{\Gamma}(\omega) = \int_0^\infty dt e^{i\omega t} \Gamma(t, 0), \quad \lim_{\omega \rightarrow 0} \tilde{\Gamma}(\omega) = \frac{1}{2}(\kappa + i\gamma). \quad (14)$$

These are often written in terms of dimensionless variables $\hat{\kappa} = \kappa/T^3$, $\hat{\gamma} = \gamma/T^3$. For chromoelectric correlators with fundamental connections that appear in the context of heavy quark diffusion, $\hat{\kappa}$ has been calculated over a wide range of T 's and is known to have a weak [33,100] T dependence, showing an increase near the critical temperature (in the pure glue theory) as it is approached from above. Here, we will assume that $\hat{\kappa}$ and $\hat{\gamma}$ are T independent.

Our goal is to go beyond these approximations and directly solve Eq. (10). Although linear, it is still formidable to solve due to the large number of degrees of freedom associated with the spatial coordinates in three dimensions. Since we will ultimately look at only states with a definite angular-momentum quantum number l , it is useful to work in the angular-momentum basis $|l, m\rangle$. An additional benefit of using this basis is that the transition rules can be written in a simpler form [14,76,79]. Furthermore, it can be shown that when the initial density matrix $\rho_S(0)$ is block diagonal in $|l, m\rangle$ basis, then for the evolution equation (10) it will be block diagonal for subsequent times. Defining the blocks by

$$\rho^l(t) = \sum_{m=-l}^l \langle l, m | \rho_S(t) | l, m \rangle, \quad (15)$$

where we have summed over the azimuthal quantum number m since we are not considering any observables that are sensitive to transitions between different m values for a given l . The evolution equation for $\rho^l(t)$ can be written

as

$$\begin{aligned} \frac{\partial \rho^l(t)}{\partial t} = & -i[h^l, \rho^l(t)] - \int_0^t ds \sum_{n,l'} (\Gamma(t, t-s) T_n^\dagger(l \rightarrow l', 0) \\ & \times T_n(l \rightarrow l', -s) \rho^l(t) - \Gamma(t, t-s) T_n(l' \rightarrow l, -s) \\ & \times \rho^{l'}(t) T_n^\dagger(l' \rightarrow l, 0) + \text{H.c.}), \end{aligned} \quad (16)$$

where

$$\begin{aligned} h^l = & \begin{pmatrix} h_s^l & 0 \\ 0 & h_o^l \end{pmatrix}, \quad \text{with} \\ h_{s,o}^l = & \frac{1}{M} \left(-\frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{l(l+1)}{r^2} \right) + v_{s,o}(r). \end{aligned} \quad (17)$$

The summations over n and l' in Eq. (16) indicate a sum over transitions between states with different color quantum numbers (s, o) and orbital angular momentum (l, l'), and the corresponding time-dependent transition operators at time t are $T_n(l \rightarrow l', t)$. To the order in pNRQCD that we are working in [Eq. (1)], only transitions between angular momentum states $l' = l \pm 1$ are allowed due to the dipole interaction. The explicit form of the transition operators is given by

$$T_n(l \rightarrow l', t) = C_{l,l'} \times \begin{cases} e^{ih_o^l t} r e^{-ih_s^l t} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ e^{ih_s^l t} r e^{-ih_o^l t} \begin{pmatrix} 0 & \sqrt{\frac{1}{N_c^2-1}} \\ 0 & 0 \end{pmatrix} \\ e^{ih_o^{l'} t} r e^{-ih_s^{l'} t} \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\frac{N_c^2-4}{2(N_c^2-1)}} \end{pmatrix} \end{cases}, \quad (18)$$

for $n = 1, 2, 3$, respectively, and $C_{l,l'}$ is given by

$$C_{l,l'} = \sqrt{\frac{l+1}{2l+1}} \delta_{l',l+1} + \sqrt{\frac{l}{2l+1}} \delta_{l',l-1}. \quad (19)$$

The master equation (16) can be given a simple interpretation similar to that of a rate equation. In Eq. (16), the first pair of T_n 's correspond to the process $l \rightarrow l' = l \pm 1 \rightarrow l$, and the second term corresponds to the contribution from the transitions $l' = l \pm 1 \rightarrow l$. There will be higher-order transitions if one goes beyond the leading-order multipole expansion.

III. NUMERICAL SIMULATION

Master equations of the form of Eq. (16) can be solved using stochastic methods such as stochastic unraveling [82]. Consider a general master equation,

$$\frac{\partial \rho_S(t)}{\partial t} = A(t)\rho_S(t) + \rho_S B^\dagger(t) + \sum_i (C_i(t)\rho_S(t)D_i^\dagger(t) + \text{H.c.}). \quad (20)$$

For Eq. (16),

$$\begin{aligned} \rho_S(t) &= \sum_l \rho^l(t) |l\rangle \langle l| \\ A(t) &= B(t) = -i \sum_l h_{\text{eff}}^l(t) |l\rangle \langle l| \\ -ih_{\text{eff}}^l(t) &= -ih^l - \int_0^t ds \Gamma(t, t-s) \\ &\quad \times \sum_{n,l'} T_n^\dagger(l \rightarrow l', 0) T_n(l \rightarrow l', -s), \\ C_n(t) &= \sum_{l,l'} \int_0^t ds \Gamma(t, t-s) T_n(l' \rightarrow l, -s) |l\rangle \langle l'|, \\ D_n(t) &= \sum_{l,l'} T_n(l' \rightarrow l, 0) |l\rangle \langle l'|. \end{aligned} \quad (21)$$

As mentioned above, equations of the form of Eq. (20) can be solved by using stochastic unraveling, which involves considering an ensemble of wave functions describing the state of the system, $\{|\psi(t)\rangle\}$, each evolving according to a stochastic equation. The stochastic equation describes continuous (albeit nonunitary) evolution of $\{|\psi(t)\rangle\}$, combined with random “jumps” of $\{|\psi(t)\rangle\}$ with probabilities governed by the operators C_i and D_i . $\rho_S(t)$ is obtained by taking an ensemble average of the outer product of $\{|\psi(t)\rangle\}$. We refer the reader to Ref. [82] for more details.

For LO [78] and NLO [34,79] Lindblad equations, it has been found previously that evolution with h_{eff}^l [Eq. (21)] is sufficient to describe the survival probability of $\Upsilon(1S)$ states, and results obtained by solving the Lindblad equation with and without jumps are very close. However, for $\Upsilon(2S)$ and $\Upsilon(3S)$ which are not as strongly bound, jumps are necessary to obtain the accurate survival probability and are essential for capturing the phenomenon of regeneration. Regeneration is a key process for obtaining a realistic phenomenological description of the suppression of the excited states [34,79]. The physical reason behind this observation is that jumps from the $1S$ states contribute significantly to the depleted number of excited states, while the reverse process is less likely.

Motivated by this observation, in this paper, we focus on $\Upsilon(1S)$ states and simplify our calculation by neglecting the jump terms [formally taking C, D to 0 in Eq. (21)]. In this approximation, the evolution is deterministic, and the evolution equation for the radial part of singlet wave function $|\psi_l, t\rangle$ is given by

$$\begin{aligned} \frac{\partial |\psi_l, t\rangle}{\partial t} &= -ih_s^l |\psi_l, t\rangle \\ &\quad - \int_0^t ds \Gamma(t, t-s) \left\{ \left(\frac{l+1}{2l+1} \right) r e^{-ih_o^{l+1}s} r e^{ih_s^l s} \right. \\ &\quad \left. + \left(\frac{l}{2l+1} \right) r e^{-ih_o^{l-1}s} r e^{ih_s^l s} \right\} |\psi_l, t\rangle, \end{aligned} \quad (22)$$

where we have assumed that the system starts as a state with a definite orbital angular momentum l . As mentioned above, in the absence of jumps, regeneration from states of higher l' deexciting to l does not play a role.

The calculation is still numerically challenging because for each value of s operators like $T_n(l \rightarrow l', -s)$ in Eq. (21) are proportional to $e^{-ih_a^l s} r e^{ih_b^l s}$. The operators of the form $e^{ih_a^l s}$ can be evaluated once in the energy basis for a range of t values of interest and saved for efficient implementation. At each time t , $T_n(l \rightarrow l', -s)$ is convolved with $\Gamma(t, s)$, and this is the most computationally challenging step when the background medium evolves with time since $\Gamma(t, s)$ depends on the evolution history of the temperature T along the trajectory of the CM of the quarkonium state.

We end this section by giving some information about the numerical implementation of Eq. (22) and some parameter values for the system. For a given l , the radial wave function is discretized in the range $[0, L_r]$ with $L_r = 6$ fm, and spacing between points is $\Delta r = 0.02$ fm. We work with the radial part of the wave function multiplied by r , as usual [101], $y_l(r) = r R_l(r)$, where $R_l(r) = \langle r | \psi_l \rangle$. We use the boundary condition that $y_l(r)$ vanishes at $r = 0$ and $r = L_r$. To make a direct comparison with the NLO results of Refs. [34,79], in this study, we take the potentials be Coulombic,

$$v_s(r) = -\frac{C_F \alpha_s}{r}, \quad v_o(r) = \frac{\alpha_s}{2N_c r}. \quad (23)$$

α_s and M (see Table I for a summary) are taken to be the same as those used in Ref. [79]. With these parameters, $E_b = 460.4$ MeV, giving $\tau_s \sim 0.4$ fm. The initial state is taken to be the $1S$ eigenstate with the singlet Coulomb potential $v_s(r)$. In Ref. [77], it is found that, for LO Lindblad evolution, initial states of a Gaussian form with widths $\sim 1/M$ and Coulombic eigenstates give the same evolution for $1S$ state. Hence, we do not investigate these systematics here.

TABLE I. Parameters of the model. α_s determines the potentials [Eq. (23)], and the choice of M and α_s was made to facilitate comparisons with Ref. [79]. We evolve the states till the medium in the neighborhood of the state reaches a temperature $T_{\min}$ (see discussion in Sec. IV).

M	α_s	$\hat{\kappa}$	$\hat{\gamma}$	$T_{\min}$
4.73 GeV	0.468	4.0	0	160 MeV

The final ingredient we need in order to evaluate $A(t)$, $B(t)$ [Eq. (21)] is $\Gamma(t, s)$. Motivated by the arguments of Appendix C, we take its form in a static medium to be

$$\Gamma(t, s) = \frac{\kappa}{2\tau_E} e^{-(t-s)/\tau_E}, \quad t > s. \quad (24)$$

Values for $t < s$ are not needed in our calculation, but the real part of Γ is symmetric under $t \rightarrow s$.

For all the results presented in this section, we use the transport coefficient values to be $\hat{\kappa} = 4.0$ and $\hat{\gamma} = 0$ [34]. $\tau_E \sim 1/T$, and we vary it in a reasonable range to explore the sensitivity of our results to this parameter. The wave function is evolved using the second-order Runge-Kutta method with step size $\delta t = 0.001$ fm, which is much smaller than τ_R as well as τ_E .

IV. RESULTS

In this section, we describe results for $\Upsilon(1S)$ suppression calculated using the method described in the previous section. Our main goal is to illustrate the dependence of suppression on the hierarchy between τ_S and τ_E . Since the binding energy and therefore τ_S are fixed, we vary τ_E . Intuitively, τ_E should scale as the inverse of the medium temperature. Therefore, we vary τ_E by changing $\xi_E = \tau_E \cdot T$. We calculate results for three different values of ξ_E : $\{1/(1.5), 1, 1.5\}$. Only in Fig. 1, we use a slightly wider range for illustrative purposes in a simple case.

We consider three different models for the hydrodynamic background. First, to understand the effect of varying τ_E in a simple setting, we will take the medium to be at a fixed temperature and see how the survival probability evolves

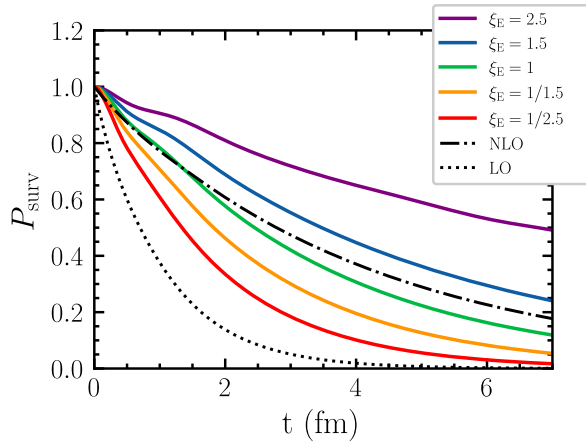


FIG. 1. The time dependence of the survival probabilities of $\Upsilon(1S)$ in a static medium at a temperature of 350 MeV. The solid curves correspond to the calculations using the master equation (16). The dotted curve (black online) corresponds to LO [77], and the dot-dashed curve (black online) corresponds to NLO [79]. $\xi_E = \{1/2.5, 1/1.5, 1, 1.5, 2.5\}$ correspond to $\tau_S/\tau_E \sim T/(\xi_E E_b) = \{1.9, 1.1, 0.8, 0.5, 0.3\}$, respectively, for $T = 350$ MeV and $E_b = 460.4$ MeV.

with time. We then consider the evolution of the survival probability in a simple Bjorken expanding medium. Finally, we show results obtained by taking the medium evolution to be described by a phenomenologically validated model of viscous 2 + 1 hydrodynamic evolution at LHC and RHIC [48,49] and compare our results for R_{AA} for $\Upsilon(1S)$ with those obtained by these experiments.

For Bjorken and hydrodynamic backgrounds, we evolve the quantum state until the medium temperature drops below $T_{\min} = 160$ MeV, close to the freeze-out temperature. We will see that the survival probability stops changing well before this, and hence increasing or decreasing $T_{\min}$ by a few MeV will not change our results for R_{AA} .

A. Static medium

In Fig. 1, we present $\Upsilon(1S)$ survival probabilities for a static background at a constant temperature of $T = 350$ MeV. Along with the five values of ξ_E , we plot LO and NLO results calculated from the effective Hamiltonian given in Ref. [79]. We observe a strong dependence of the survival probabilities on ξ_E and therefore on the value of the τ_S/τ_E , keeping T and hence κ fixed.

Let us first consider the difference between the results obtained by solving the master equation (solid curves in Fig. 1) and LO (dotted black curve in Fig. 1). The suppression using LO is much larger. This can be understood from Eq. (2). The spectral function corresponding to Eq. (24) can be approximated by the form [54]

$$\frac{\rho(\omega)}{\omega} \sim \frac{\kappa \Omega^2}{(\omega^2 + \Omega^2)T}, \quad (25)$$

with $\Omega = 1/\tau_E$. The LO calculation corresponds to assuming $\Omega \gg E_b$, in which case one can set $\omega \sim E_b = 0$ in Eq. (25). However, for $\omega \sim E_b = 460$ MeV and $\Omega \sim T = 350$ MeV, the r.h.s. of Eq. (25) is smaller than its zero-frequency value, leading to higher survival probability [18,83].

The relative suppression for the three ξ_E values in Fig. 1 is also clear from the above argument. Increasing Ω keeping T , κ and E_b unchanged will lead to a larger suppression, with $\Omega \rightarrow \infty$ corresponding to the LO result.

We can also anticipate the effect of increasing T keeping ξ_E and E_b unchanged. The overall suppression will increase for all the calculations, because of a larger κ . However, we expect the LO and the master equation to be relatively closer together, corresponding to a smaller E_b/Ω . The opposite effect is expected if we decrease T . Detailed calculations bear out this intuition. We have relegated these results to Fig. 5 in Appendix B. The trend is as expected.

Now, we consider the results of the NLO calculation (dot-dashed black curve in Fig. 1). As expected, the NLO corrections capture the effect of a finite E_b/T . It is interesting that for $T = 350$ MeV, and $\xi_E = 1$, the NLO results lie very close to the result from the master equation, especially after about 2 fm when the transient oscillations in

the master equation have died down. However, this is a numerical coincidence. Based on the argument above, we expect the NLO results to lie closer to results from the master equation with a larger ξ_E if we increase T . This is because we expect the NLO calculation to capture the dynamics for longer environmental relaxation times (E_b/T is smaller). Similarly, for a smaller T , we expect NLO results to be closer to results from the master equation with a smaller ξ_E . This trend is seen in Fig. 5 in Appendix. B.

It is worth remarking on the transient oscillations in the survival probability seen at early times in the solution of the master equation. These arise from the convolution of $e^{\pm i(h_s - h_o)t} \sim e^{\pm iE_b t}$ with e^{-t/τ_E} and decay after a few τ_E .

B. Bjorken background

In this section, we analyze the evolution of the survival probability as a function of time in a Bjorken expanding medium with a temperature evolution given by

$$T(\tau) = T(\tau_0) \left(\frac{\tau_0}{\tau} \right)^{\frac{1}{3}}, \quad (26)$$

where τ_0 is the initial time of the start of hydrodynamic evolution. In Fig. 2, we show two plots for the survival probability of $\Upsilon(1S)$ with initial temperatures $T(\tau_0)$ 480 and 333 MeV. The values of τ_0 are 0.6 and 1.0 fm, respectively. These temperatures and times correspond to the typical values in the most central collisions at 5.02 TeV and 200 GeV energies [18,102]. As in the static case, we show the survival probability for three values of $\xi_E \in \{1.5, 1, 1/1.5\}$. Along with these curves, we plot the LO and NLO probabilities.

We consider $\Upsilon(1S)$ states at rest in the medium or moving slowly at central rapidity in the medium, and hence t in Eq. (16) is the same as τ . The T at time t needed for estimating Γ is obtained from Eq. (26). However, there is a subtlety in determining $\Gamma(t, s)$ in the evolving medium

since $\Gamma(t, s)$ is sensitive to temperatures over a time interval τ_E around t and modeling $\Gamma(t, s)$ requires further assumptions. In fact, in principle $\Gamma(t, s)$ is not necessarily a function only of $t - s$. However, here we assume that the evolution is slow enough that $\Gamma(t, s)$ still has the form given by Eq. (24) with the change that κ is given by $\hat{\kappa} \left(\frac{T(t) + T(s)}{2} \right)^3$ and τ_E given by

$$\tau_E(t, s) = \xi_E \left(\frac{2}{T(t) + T(s)} \right). \quad (27)$$

We have seen in a simple case that using $T(t)$ instead of the average of $T(t)$ and $T(s)$ changes the result by less than the range obtained by using $\xi_E \in \{1/1.5, 1.5\}$. We leave a more detailed analysis of this systematic for future work.

The relative order (Fig. 2) between the results obtained from the master equation and the results from the LO and the NLO calculations is similar to those observed and described in Sec. IV A. However, there are a few additional features to highlight.

First, in contrast to the static medium, the survival probabilities in the master equation change very gradually after about $t \sim 8$ fm at the LHC and $t \sim 5$ fm (corresponding to $T \sim 200$ MeV in both cases). (This is not an artifact of the choice of the prescription equation (27), since, for example, using $T(t)$ to determine the environment correlator will lead to an even smaller decay probability at late times.)

It simply stems from the fact that, for a given ξ_E at small T , $\omega/\Omega \sim E_b/\Omega$ is large, and the factor $\Omega^2/(\omega^2 + \Omega^2)$ in Eq. (25) is smaller. This further reduces the probability of decay, on top of the overall reduction in the strength of Γ due to a smaller κ .

This effect is absent in LO. In fact, for the RHIC with the parameters above, the decay probability remains substantial for LO even at 6 fm. As anticipated in Sec. IV A, while the NLO calculation captures this effect at high T , at low T (late times), the NLO calculation is expected to break

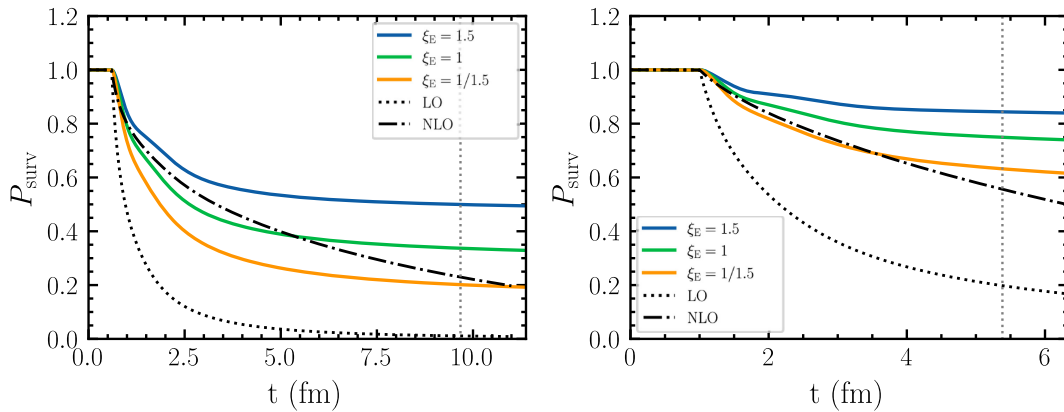


FIG. 2. $\Upsilon(1S)$ survival probabilities as a function of time in Bjorken expanding media with $(t_0, T(t_0))$ taken to be (0.6 fm, 480 MeV) (left panel) and (1.0 fm, 333 MeV) (right panel). The vertical line corresponds to the time at which the temperature drops below 190 MeV, which corresponds to the $T_{\min}$ used for NLO simulations in Ref. [79]. The choice of the style of curves is the same as Fig. 1.

down and receive large corrections from higher-order correction terms in the E_b/T expansion. The effect is more pronounced at RHIC because of the smaller T . This late-time behavior is tamed in Refs. [34,79] by taking a larger $T_{\min} \sim 190$ MeV.

C. Realistic hydrodynamic background

In this section, we present the results for $\Upsilon(1S)$ suppression for 200 GeV Au-Au and 5.02 TeV Pb-Pb collisions. Results for 2.76 TeV Pb-Pb collisions are similar to 5.02 TeV Pb-Pb collisions and are shown in Appendix D. We take the evolution of the background thermal medium to be given by the model used for the phenomenology of light hadrons at the RHIC and LHC [48,49]. In this model, for a given impact parameter b , the initial distribution of nucleons is given by the Glauber model [103], and the collision and the initial dynamics are described by a multi-phase transport model (AMPT) [104]. This is coarse grained into a hydrodynamic state, which is evolved using $(2+1)$ -dimensional viscous hydrodynamics. The transport coefficients are tuned to fit the spectra of soft particles.

For each decile of centrality bins, we sample $10b$'s from the distribution given by the Glauber model. For a given b , the hydrodynamic simulation provides the temperature profile of the medium as a function of position and time. The model incorporates initial-state fluctuations since it uses fluctuating Glauber initial conditions and since the transport model AMPT is probabilistic, and hence for each b value, we use five different hydrodynamic realizations and average over them to obtain our results.

For a given hydrodynamic realization, the $\Upsilon(1S)$ can move along various trajectories. In pNRQCD, the CM dynamics decouples from that of the relative motion of the $Q - \bar{Q}$, and since bottomonia do not get strong enough kicks from the medium for it to alter the CM trajectory, each trajectory is taken to be a straight line. The trajectory is fixed by the initial conditions: position (x_0, y_0) ,

transverse momentum p_T , and direction of velocity given by the azimuthal angle ϕ with respect to the reaction plane in the Glauber model. We assume that the generated quarkonia have zero momentum rapidity. Therefore,

$$(x(t), y(t)) = (x_0, y_0) + t \frac{p_T}{E} (\cos(\phi), \sin(\phi)), \quad (28)$$

where p_T is the transverse momentum and E the energy.

The production points (x_0, y_0) of the quarkonium are sampled from the distribution of binary collisions,

$$N_{\text{bin}}(x, y, b) = T_{AB}(x, y, b) \sigma_{\text{in}}^{\text{NN}}, \quad (29)$$

where $\sigma_{\text{in}}^{\text{NN}}$ is the nucleon-nucleon inelastic cross section and T_{AB} is the overlap distribution. The velocity angle ϕ is sampled uniformly from the interval $[0, 2\pi)$.

The transverse momentum is sampled from the distribution

$$P(p_T) = \frac{2M_{Q\bar{Q}}^2 p_T}{(p_T^2 + M_{Q\bar{Q}}^2)^2}, \quad (30)$$

where $M_{Q\bar{Q}}$ is the mass of the quarkonium under consideration. For a given impact parameter, we sample 2000 trajectories.

The quarkonium state experiences a time-dependent temperature as it moves through the medium along a trajectory obtained as described above. For a given trajectory, the temperature is given as a function of time by the hydrodynamic realization. This determines the correlator $\Gamma(t, s)$ according to Eq. (27).

In Fig. 3, we show the final survival probability P_{surv} for $\Upsilon(1S)$ in 5.02 TeV Pb-Pb and 200 GeV Au-Au collisions. The impact parameters are binned into centrality classes, and P_{surv} is plotted for each centrality bin as a function of the averaged N_{part} . As in the case of static and Bjorken

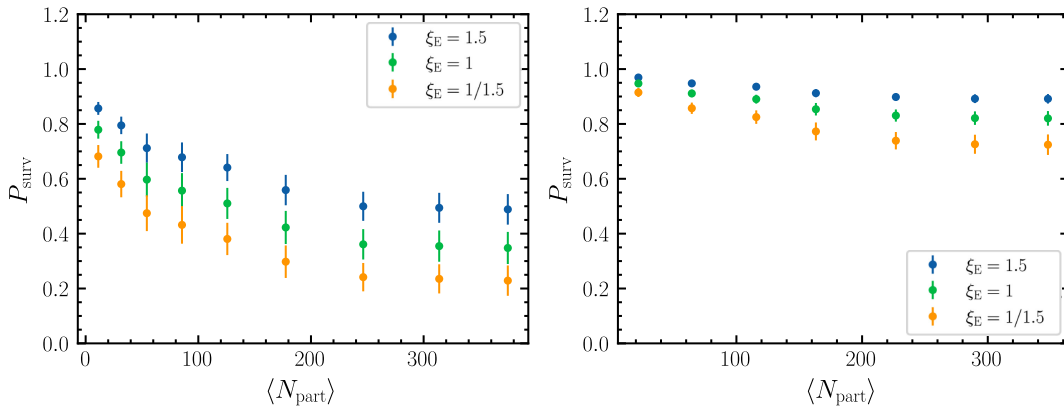


FIG. 3. Final survival probability as a function of $\langle N_{\text{part}} \rangle$ for $\Upsilon(1S)$ with a viscous hydrodynamic background for Pb-Pb collisions at 5.02 TeV (left) and Au-Au collisions at 200 GeV (right). In each plot, three sets of results corresponding to $\xi_E = \{1.5, 1, 1/1.5\}$ are shown which were obtained from the master equation (16). The error bars correspond to the statistical errors from the sampling of quarkonium trajectories.

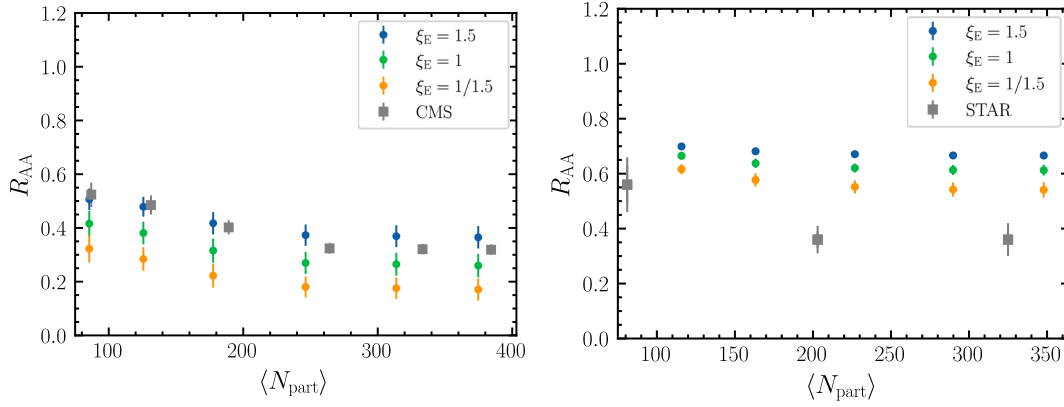


FIG. 4. R_{AA} as a function of $\langle N_{part} \rangle$ for $\Upsilon(1S)$ in Pb-Pb collisions at 5.02 TeV (left) and Au-Au collisions at 200 GeV energy (right) after estimating the feed-down contributions as discussed in the text. Experimental data from CMS [105] and STAR [92] are plotted for comparison. Data from ATLAS [88] at 5.02 TeV are consistent with the CMS data and are not shown here for cleaner plots.

backgrounds, there is a strong dependence of the suppression on ξ_E .

For a comparison with the experimental data, late-time feed-down must be included. For more central collisions, we can make a rough estimate of the contributions from feed-down. Since the direct contribution to $\Upsilon(1S)$ state is about 75% [77], if we assume that for $N_{part} \gtrsim 80$ all the excited states [in particular $\chi_{b0}(1P)$ and $\chi_{b1}(1P)$] are much more suppressed (a plausible hypothesis based on the observed R_{AA} of $\Upsilon(2,3S)$ [86,88,105]), then the R_{AA} for $\Upsilon(1S)$ can be roughly estimated from our results in Fig. 3, by scaling them by 0.75, and this is shown in Fig. 4 for the LHC (left) and RHIC (right).

The model agrees with the experimental data at LHC energies (also see Fig. 7 in Appendix. D) for reasonable values of ξ_E . RHIC measurements of the $\Upsilon(1S)R_{AA}$ indicate the same degree of suppression as obtained for LHC energies. Intuitively, one would expect a lower suppression due to the lower temperatures of the QGP produced at the RHIC. Our values underestimate the $\Upsilon(1S)$ suppression compared to the experimental values.

We note that one can reconcile the two measurements by taking ξ_E to be around 1.5 at the LHC and even smaller than 1/1.5 at the RHIC. However, a reduction of ξ_E at the RHIC by a factor of over 2.3 is not very easy to understand, and hence we surmise that additional effects may need to be taken into account to get to a realistic phenomenology. Some of these have been listed in the Introduction.

For example, we have not considered the initial- and final-state cold nuclear matter effects such as nuclear absorption, which might give additional contributions to the observed suppression. The results from Ref. [106] indicate that nuclear absorption may play a role at 200 GeV energies.

Another effect that might play a role in understanding the larger-than-expected suppression observed at the RHIC could be an increase in $\hat{\kappa}$ as T approaches the crossover temperature from above [see the discussion below Eq. (14)]. This may play a more important role at the RHIC than at the LHC because of the overall lower temperature of the medium.

V. CONCLUSIONS

We solve non-Markovian master equations for the evolution of the $\Upsilon(1S)$ state in the QGP. For $\tau_E/\tau_S \rightarrow 0$, these equations reduce to LO Lindblad equations. To study the dependence on τ_E ($\tau_S \sim 1/E_b$ is fixed), we analyze the survival probability of $\Upsilon(1S)$ for $\tau_E = \xi_E/T$ for three values of ξ_E : $\xi_E = \{1/1.5, 1, 1.5\}$. We find that as ξ_E decreases the survival probability decreases, but for all $\xi_E \sim 1$, LO [77,78] Lindblad equations significantly overestimate the suppression of $\Upsilon(1S)$ (see. Figs. 1 and 2).

We find that the NLO [34,79] equations capture much of this reduction of the suppression for realistic ξ_E at T 's well above the crossover temperature, but our calculations in Bjorken backgrounds (Fig. 2) suggest that at temperatures $\lesssim 250$ MeV the NLO equations do not agree with non-Markovian master equations suggesting higher-order corrections might be necessary. R_{AA} values found using the non-Markovian master equation are not very sensitive to the choice of the freeze-out time of the $\Upsilon(1S)$, as long as it is roughly around 200 MeV or below. (Interestingly, temperatures of about 200 MeV are not inconsistent with the extraction of the freeze-out time for bottomonium states from statistical models [107,108].)

The key ingredient in our calculation is the chromoelectric correlator whose overall strength is governed by the transport coefficient κ [Eq. (14)] (we take $\gamma = 0$). From our results, one can see that a larger τ_E can be compensated for by a larger κ , and hence an independent determination of κ is needed to narrow down the parameter space in the absence of other independent observables in this sector.

Using a realistic hydrodynamic medium for the RHIC (right) and LHC (left) in Fig. 4, we find the final probability of survival of the $\Upsilon(1S)$ states in these experiments. While a smaller “effective” ξ_E might partly explain the suppression observed at the RHIC, there is room for additional effects. We leave a more detailed attempt at phenomenology for future work.

Finally, an obvious next step can be including jumps and addressing the phenomenology of the excited bottomonium states and their feed-down.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

APPENDIX A: LO MARKOVIAN APPROXIMATION

In this section, we review how the master equation, Eq. (8), can be rewritten as a LO Markovian equation if $\tau_E \ll \tau_S$.

The environmental correlation functions $\Gamma_{mn}(t, s)$ in Eq. (8) decay on timescales $t - s \sim \tau_E$. If this timescale is short compared to the timescale of the variation of $\mathbf{V}_S^n(s)$ (τ_S) and the observation time (t), then in the r.h.s. of Eq. (8), the lower limit of the s integration can be set to $-\infty$ and the variation of $\mathbf{V}_S^n(s)$ can be ignored (LO in τ_E/τ_S). This is known as the Markovian approximation. In this approximation, the integral in s simply gives the 0 frequency limit of $\Gamma_{mn}(t)$, and the r.h.s. of Eq. (8) has a structure,

$$-\sum_{m,n} \tilde{\Gamma}_{m,n}(0) (\mathbf{V}_S^m(0) \mathbf{V}_S^n(0) \rho_S(t) - \mathbf{V}_S^m(0) \rho_S(t) \mathbf{V}_S^n(0)) + \text{H.c.}, \quad (\text{A1})$$

where H.c. is the Hermitian conjugate of the operator in the previous line.

The form in Eq. (A1) is not an accident. Going to the Schrödinger picture and defining a new set of operators L_k by taking appropriate linear combinations of $\mathbf{V}_S^n$, Eq. (3) in the Markovian approximation can be rewritten in a more familiar form,

$$\frac{\partial \rho_S(t)}{\partial t} = -i[H_h, \rho_S] + \sum_k \left(L_k \rho_S L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho_S\} \right), \quad (\text{A2})$$

where H_h gives the Hermitian evolution of ρ_S and L_k is a set of operators that encode its non-Hermitian evolution in a trace-preserving manner. The evolution of the state depends only on the state at that instant, and the evolution operator does not depend on the history. Equation (A2) is the well-known Lindblad form. For the specific forms of H_h and L_k calculated for quarkonia under various assumptions, we refer the reader to Refs. [54,55,71,79,109].

The physical picture behind the mathematical form above is that if $\tau_E \ll \tau_S$, any memory of the S – E exchanges is quickly lost, and the S evolution is Markovian, and it is known that any positive definite, trace-preserving, Markovian equation for the time derivative of ρ_S can be written as a Lindblad equation [59,60].

APPENDIX B: EFFECT OF T ON THE EVOLUTION FOR A STATIC MEDIUM

In this section, we show results for the survival probability as a function of time for the $\Upsilon(1S)$ state in a static medium at temperatures $T = 250$ (left) and 450 MeV (right) (Fig. 5).

Comparing these with Fig. 1 in Sec. IV A, we notice the following pattern. As T is increased, the overall

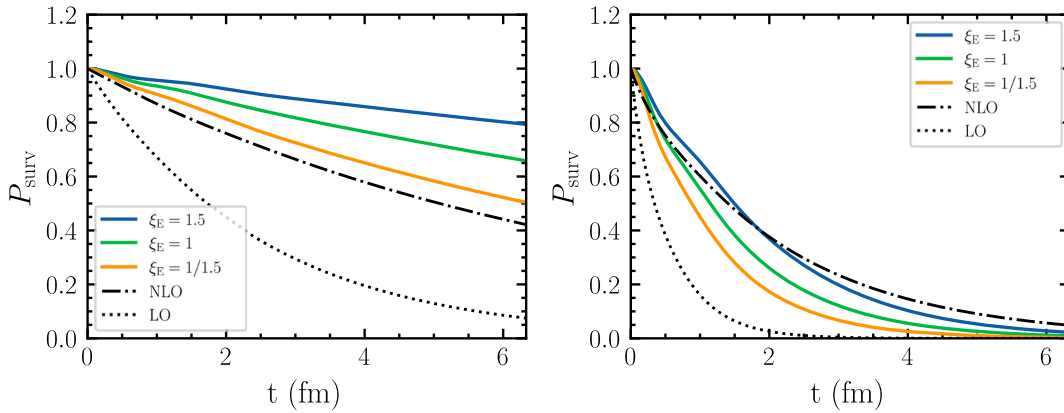


FIG. 5. Static medium at $T = 250$ MeV (left) and $T = 450$ MeV (right).

suppression increases for all the master equations since κ increases. Comparing the NLO calculation with the master equation, we note that the NLO calculation comes closer to the solution of the master equation with a larger ξ_E , as T is increased.

APPENDIX C: CHROMOELECTRIC CORRELATOR IN THE HARD THERMAL LOOP APPROXIMATION

The chromoelectric correlator, $\Gamma(t)$ [Eq. (12)], in a deconfined medium at temperature T governs the evolution of the quarkonium density matrix in the QGP. Since it is a real-time quantity, it is challenging to compute nonperturbatively using lattice QCD. Nonetheless, significant progress has been made in understanding this object. The real and imaginary parts of the zero-frequency limit of the (causal) correlator define two important transport coefficients [79,109], κ and γ , defined in Eq. (14).

One can estimate [110] γ using the shift in the peak of the quarkonium spectral function computed on the lattice [111]. More recent lattice results [112] for the shift suggest that $\hat{\gamma}$ [35] for temperatures of a few 100 MeV is small. This motivates us in this study to ignore the imaginary part of $\Gamma(t, 0)$, an assumption worth closer investigation in the future. The direct computation of $\hat{\gamma}$ is an open problem.

Similarly, a nonperturbative calculation of $\hat{\kappa}$ is an open problem. A related quantity, the heavy quark momentum diffusion constant, is defined as

$$\kappa_F = \frac{g^2}{3N_c} \int dt \text{Tr}_E(\mathcal{U}(-\infty, t; \vec{0}) \mathbf{E}(t, \vec{0}) \mathcal{U}(t, 0; \vec{0}) \times \mathbf{E}(0, \vec{0}) \mathcal{U}(0, \infty; \vec{0})), \quad (\text{C1})$$

where $\mathbf{E} = \mathbf{E}^a t^a$ and $\mathcal{U}(t_1, t_2; \vec{r})$ is the fundamental Wilson line from time t_2 to t_1 at the spatial location $\vec{r}$. This has been computed on the lattice [113,114]. (See Refs. [33,100,115–117] for more recent results.)

It is well known that the leading order (in the strong coupling g) perturbative [118,119] estimate of κ_F in the QGP phase is roughly an order of magnitude smaller than the nonperturbative result [113,114]. The next-to-leading-order result [120,121] is closer, but the large correction suggests that the series in g converges slowly for temperatures of interest for heavy ion phenomenology (150–500 MeV).

Little is known about Γ at finite frequency nonperturbatively. Therefore, it is useful to gain insight from weak-coupling approaches, even though we do not expect these approaches to be quantitatively reliable. Formally,

$$\Re[\Gamma(t, 0)] = \frac{g^2 C_F}{3} \int \frac{d^4 q}{(2\pi)^4} e^{-iq^0 t} \frac{e^{q^0/T}}{e^{q^0/T} - 1} \rho(q^\mu), \quad (\text{C2})$$

where $C_F = (N_c^2 - 1)/(2N_c)$ is the color factor and $\rho(q^\mu)$ is the chromoelectric spectral density.

In the Hard Thermal Loop (HTL) formalism at leading order [122], the contribution to the spectral density from longitudinal gluons is

$$\rho(q^\mu) = \frac{\pi m_D^2 q q^0}{(q^2 + m_D^2)^2 + (\pi m_D^2 q^0/2q)^2}, \quad (\text{C3})$$

where $m_D \sim gT$ is the screening mass.

Performing the q^0 integration in Eq. (C2) via contour integration for $t > 0$, the integrand in the lower complex plane picks residues from the pole of ρ [$q^0 = -i2q(q^2 + m_D^2)/m_D^2$ in HTL] and the residues from the poles of the Bose-Einstein distribution ($q^0 = -i2n\pi/T$, for integral $n \geq 1$). The real part of the result, therefore, has the form

$$\begin{aligned} \Re[\Gamma(t, 0)]_{\text{HTL}} &= \int \frac{d^3 q}{(2\pi)^3} q^3 \left\{ \exp[-2tq(q^2 + m_D^2)/(\pi m_D^2)] \right. \\ &\quad \times \frac{q^2 \cot[q(q^2 + m_D^2)/(\pi m_D^2 T)]}{\pi m_D^2} + \sum_{n \geq 1} \exp[-2tn\pi T] \\ &\quad \times \left. \frac{2\pi^2 q^3 m_D^2 n T^2}{-q^6 - 2k^4 m_D^2 - k^2 m_D^4 + \pi^4 m_D^4 n^2 T^2} \right\}. \end{aligned} \quad (\text{C4})$$

The terms in the sum [second term in Eq. (C4)] fall off with t as $\exp[-2tn\pi T]$, while the contribution from the pole of ρ [first term in Eq. (C4)] falls off as $\sim \exp[-m_D t]$ for $q \sim m_D$ and is the dominant contribution in weak coupling when $m_D \ll \pi T$. For $g \gtrsim 1$, both the first and the second terms decay on a timescale $\sim 1/T$. Finally, it is easy to verify that [123]

$$\int_0^\infty dt \Re[\Gamma(t, 0)]_{\text{HTL}} = \frac{1}{2} \int \frac{d^3 q}{(2\pi)^3} \frac{q m_D^2 \pi T}{(q^2 + m_D^2)^2} = \frac{1}{2} \kappa_{\text{HTL}}. \quad (\text{C5})$$

This motivates our choice of the time-dependent form of the correlator,

$$\Gamma(t, 0) = \frac{\kappa}{2} \frac{e^{-t/\tau_E}}{\tau_E}, \quad t > 0, \quad (\text{C6})$$

with $\tau_E \sim 1/T$, a simple form which satisfies the integral constraint equation (14) and captures the expected exponential decay of the correlator. We note that $\Gamma(t, 0)$ will have an imaginary part [124], even if one takes $\gamma = 0$ as we do in our paper. However, we simplify our calculation by neglecting this.

APPENDIX D: $\Upsilon(1S)$ SUPPRESSION AT 2.76 TEV

In this section, we show results for the $\Upsilon(1S)$ suppression in the presence of a viscous hydrodynamic background

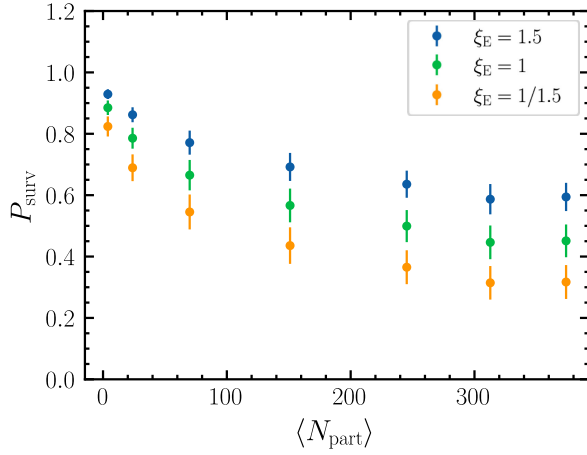


FIG. 6. Survival probability as function of $\langle N_{\text{part}} \rangle$ for $\Upsilon(1S)$ with a viscous hydrodynamic background for Pb-Pb collisions at 2.76 TeV.

for Pb-Pb collisions at 2.76 TeV energies. In Fig. 6, we show the final survival probabilities, P_{surv} , as a function of $\langle N_{\text{part}} \rangle$. As in Fig. 3, feed-down contributions at late time are not included in this plot.

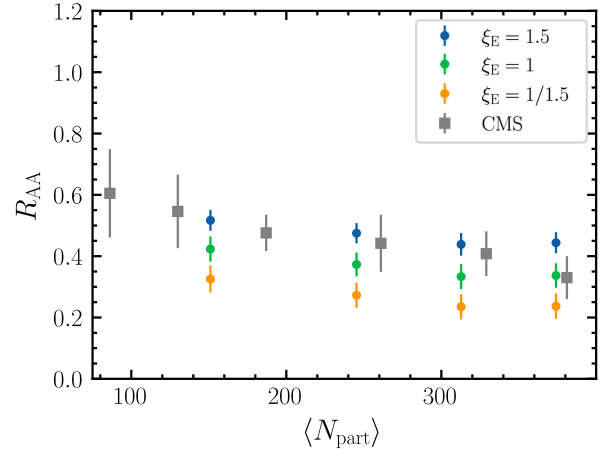


FIG. 7. R_{AA} as a function of $\langle N_{\text{part}} \rangle$ for $\Upsilon(1S)$ after estimating the feed-down contributions in Pb-Pb collisions at 2.76 TeV energy as discussed in Sec. IV C. Experimental data from CMS [86] are plotted for comparison.

Following the discussion in Sec. IV C about the estimation of feed-down contributions, we show in Fig. 7 the R_{AA} obtained by scaling P_{surv} by 0.75.

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