

Simulation of heavy quarkonium equilibration in the quark-gluon plasma

Shouxing Zhao[✉] and Min He^{✉*}

Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, China



(Received 20 August 2025; accepted 20 October 2025; published 12 November 2025)

We simulate the heavy quarkonium equilibration through transport in a static and homogeneous quark-gluon plasma (QGP) box within the semiclassical Boltzmann approach, incorporating both the leading-order and next-to-leading-order dissociation and regeneration reactions. The scattering amplitudes involved are taken from perturbative computations based on effective color-electric dipole coupling of the heavy quarkonium with thermal gluons. By coupling the Langevin simulation of single heavy quark diffusion and the Boltzmann transport of the heavy quarkonium in a real-time fashion, we demonstrate how the kinetic and chemical equilibrium of heavy quarkonium with single heavy quarks in the medium is achieved in terms of both the bound state's yields and momentum distributions. The pertinent equilibration time turns out to be comparable to the lifetime of the QGP created in the most central heavy-ion collisions at the LHC energies. The role of the intricate interplay between the open and hidden heavy sector in the process of equilibration is highlighted. This work provides a dynamical way of understanding the phenomenological success of the statistical hadronization model for charmonium production in relativistic heavy-ion collisions and also paves the way for realistic phenomenological applications to heavy quarkonium transport.

DOI: [10.1103/4rdc-9dkx](https://doi.org/10.1103/4rdc-9dkx)

I. INTRODUCTION

Heavy quarkonia below the open heavy-meson threshold are considered to be nonrelativistic bound states of charm (c) and bottom (b) quark-antiquark pairs, as primarily justified by the large quark masses $m_{c,b} \gg \Lambda_{\text{QCD}}$. While the vacuum spectroscopy of these bound states represent a versatile laboratory for testing the pertinent binding force, the spectral and abundance modifications of heavy quarkonia in the quark-gluon plasma (QGP) environment as created in relativistic heavy-ion collisions provide useful probes of the color force and transport properties of the deconfined medium [1–3]. In this regard, the primary observation was the weakening of the in-medium heavy quark potential due to the Debye screening of the static color charge surrounded by liberated thermal partons, which eventually leads to the melting of bound states at sufficiently high temperatures [4,5]. As a result, the heavy quarkonium yield in heavy-ion collisions would be suppressed compared to that produced in proton-proton (pp) collisions and scaled by the hard binary collision number, which has been corroborated in particular, by the

suppression pattern of $\Upsilon(nS)$ (s wave $b\bar{b}$ bound states) mesons in the sequence of their vacuum binding energies [6]. It has been argued in the statistical hadronization model that color screening might melt all initially produced charmonia and therefore the final production of charmonia is simply given by their statistical equilibrium yields [7–9].

The heavy quarkonium in-medium dynamics turns out much richer than the pure static screening picture. First, the transitions from bound states to unbound heavy quark pairs, i.e., dissociation caused by the dynamical scattering off the medium partons, can reduce the heavy quarkonium yield. The dissociation reactions include the $2 \rightarrow 2$ gluodissociation (also known as leading-order dissociation) $\Psi + g \rightarrow Q + \bar{Q}$ [Ψ denotes a heavy quarkonium and $Q(\bar{Q})$ the heavy quarks] and the $2 \rightarrow 3$ partonic inelastic scattering (also known as next-to-leading-order dissociation) $\Psi + p \rightarrow Q + \bar{Q} + p$ with thermal partons $p = g, q/\bar{q}$. The former is analogous to the photodissociation of neutral atoms via a dipole transition and has long been studied since the seminal work by Peskin [10,11]. The latter, as first proposed in [12] from the “quasifree” perspective, overcomes the phase-space mismatch inherent in the gluodissociation process when the incident gluon energy is significantly larger than the bound state binding energy. This $2 \rightarrow 3$ process has since also been intensively studied from the dynamical scattering point of view [13–17] and from the Landau damping (or imaginary potential) point of view [18–20]. Inverse to the dissociation process, the quarkonium bound state can be regenerated via recombination of single Q and $\bar{Q}$ near in phase space

*Contact author: minhephys@gmail.com

Published by the American Physical Society under the terms of the [Creative Commons Attribution 4.0 International license](https://creativecommons.org/licenses/by/4.0/). Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI. Funded by SCOAP³.

[21–23], in particular, in situations where there are multiple heavy quark pairs diffusing and thermalizing in the QGP, e.g., charm production in Pb-Pb collisions at the LHC energy. The regeneration production of charmonia and B_c mesons has been corroborated by the experimental observations of the significant enhancement of the yields of these bound states at low transverse momenta p_T and the J/ψ large elliptic flow [24–26] and the pertinent theoretical explanations [27–30].

A natural theoretical framework to simultaneously incorporate dissociation and regeneration dynamics and thus to simulate the heavy quarkonium transport in the QGP is the semiclassical Boltzmann equation [31]. Various forms of this approach have been implemented in literature, considering only the $2 \leftrightarrow 2 \Psi + g \leftrightarrow Q + \bar{Q}$ process [27,32], including also the $2 \leftrightarrow 3 \Psi + p \leftrightarrow Q + \bar{Q} + p$ reactions [33–36] or via the reduced rate equation [37]. A more modern treatment of the heavy quarkonium transport is the open quantum system (OQS) approach [38–40]. The OQS approach keeps track of the evolution of the $Q\bar{Q}$ pair wave packet in a hot medium via the Lindblad equation and takes care of the quantum transitions between different eigenstates. However, solving the Lindblad equation is numerically expensive and currently it is limited to the simulation of the dynamics of only one correlated $Q\bar{Q}$ pair [41–44]. In the quantum optical limit (relatively low temperature where quarkonia are still tightly bound), it was demonstrated that the semiclassical Boltzmann equation can be derived from the OQS approach [40,45].

Given the complex nature of these transport approaches (various theoretical approximations involved, interplay between the microscopic reactions and macroscopic evolutions, and coupling the heavy quarkonium system to the dynamically expanding QGP background, etc.), it is theoretically desirable to investigate some limiting cases of heavy quarkonium transport even under simplified conditions, in order to ensure that the transport implementations work properly and basic principles check out before embarking on real phenomenological applications. In this respect, it is principally important to theoretically delineate and numerically demonstrate how the heavy quarkonium kinetic and chemical equilibration occurs should the system be given long enough time to evolve, which is not only interesting in its own right, but may also unravel in a dynamical way the rationale underlying the phenomenological success of the statistical hadronization model for describing the production of charmonia [7–9] and B_c mesons [30] in Pb-Pb collisions at the LHC energy. This is exactly the purpose of the present work.

The simulation of heavy quarkonium equilibration has been previously pursued using semiclassical Langevin [46,47] or Boltzmann transport [32] and the OQS approach [43,44]. Distinct from these works that are limited to color-singlet attractive potential, $2 \leftrightarrow 2$ reactions, or one pair of

correlated $Q\bar{Q}$, we simulate the heavy quarkonium equilibration via the Boltzmann equation incorporating both the $2 \leftrightarrow 2 \Psi + g \leftrightarrow Q + \bar{Q}$ and $2 \leftrightarrow 3 \Psi + p \leftrightarrow Q + \bar{Q} + p$ reactions, with pertinent realistic scattering amplitudes computed from our previous work [17,48]. Limiting our consideration to a finite number of $Q\bar{Q}$ (more specifically, ten pairs of c and $\bar{c}$ quarks resembling the realistic case in central Pb-Pb collisions at the LHC energies) and one species of heavy quarkonium (specifically, the ground state charmonium J/ψ) in a static and homogeneous QGP box, while coupling the dissociation/regeneration reactions of the J/ψ with the Langevin diffusion of single c quarks, we keep track of the time evolution of the yields as well as the momentum distributions for the bound state. We are able to demonstrate that, although lagging behind and dependent on the thermalization of single c quark kinetics, the dissociation and regeneration dynamics always drives the J/ψ yields toward relative chemical equilibrium with the open c and $\bar{c}$ quarks in the box as dictated by the statistical balance equation [8], and the J/ψ momentum distributions also come to thermal equilibrium, irrespective of the initial conditions explored. In particular, catalysislike $2 \leftrightarrow 3$ reactions are shown to accelerate the heavy quarkonium equilibration at high temperatures due to their larger reaction rates compared to the $2 \leftrightarrow 2$ processes [14,17]. This study not only lays a solid foundation for phenomenological applications, but also highlights the interplay between open and hidden charm transport, especially through the off-diagonal (i.e., originating from different primordial hard partonic scatterings) recombination of c and $\bar{c}$ quarks forming bound state charmonium, thus reiterating the findings previously obtained in the context of addressing the J/ψ 's large elliptic flow [28].

This article is structured as follows. In the subsequent Sec. II, the microscopic reactions that underlies the heavy quarkonium dissociation and regeneration dynamics are discussed, where the transition amplitudes serving as input for the transport equation are illustrated. In Sec. III, we first spell out the equilibrium limit as dictated by the statistical balance between open c and $\bar{c}$ quarks and the charmonium bound state (J/ψ). Then we move on to discuss the formalism of the Boltzmann transport; in particular, the implementation of dissociation and regeneration are discussed in detail in connection with the $2 \leftrightarrow 2$ and $2 \leftrightarrow 3$ reactions we have considered. Section IV is devoted to the numerical simulations and results, where the heavy quarkonium equilibration is first simulated assuming fully thermalized c and $\bar{c}$ quarks, which is then generalized to the more general initial heavy quark distributions by coupling the single c 's diffusion via Langevin simulation to the Boltzmann transport of J/ψ . For both cases, precise relative chemical equilibrium of J/ψ with open c and $\bar{c}$ quarks are shown to be finally well reached. We summarize in Sec. V.

II. CHEMICAL REACTIONS OF QUARKONIUM IN QGP

The chemical reactions of heavy quarkonium leading to the dissociation and regeneration in the QGP are discussed in this section, including leading-order (LO, $2 \leftrightarrow 2$) and next-to-leading-order (NLO, $2 \leftrightarrow 3$) processes. The LO reaction occurs through absorbing or inversely radiating a real thermal gluon, $\Psi + g \leftrightarrow Q + \bar{Q}$, which dominates at low temperatures when the binding energy is larger than the screening mass of the medium [48]. At high temperatures, the NLO inelastic scattering processes ($\Psi + p \leftrightarrow Q + \bar{Q} + p$ with $p = g, q/\bar{q}$) become important because of new phase space being opened up [12,17]. The scattering amplitudes of these processes can be computed by identifying the transition matrix element from the $Q\bar{Q}$ color-singlet state $|S\rangle$ to an octet state $|O, a\rangle$ (a denotes the color indices) based on the gauge-invariant color-electric dipole coupling of the compact quarkonium with external soft gluons [49–51]

$$\langle O, a | V_{SO} | S \rangle = \frac{g_s}{\sqrt{2N_c}} \vec{E}^a(t, \vec{x}) \cdot \langle O | \vec{r} | S \rangle, \quad (1)$$

where $\vec{E}^a$ denotes the color-electric field, r the relative distance between Q and $\bar{Q}$, and g_s the strong coupling constant.

Using the above transition matrix element supplemented by a standard three-gluon or quark-gluon vertex, we have calculated the transition amplitudes for the LO and NLO dissociation processes within the framework of old-fashioned quantum-mechanical perturbation theory

$$\begin{aligned} T_{fi} &= \langle f | H_{\text{int}} | i \rangle + \sum_m \frac{\langle f | H_{\text{int}} | m \rangle \langle m | H_{\text{int}} | i \rangle}{E_i - E_m + i\epsilon} \\ &= T_{fi}^{\text{LO}} + T_{fi}^{\text{NLO}}. \end{aligned} \quad (2)$$

for a heavy quarkonium sitting at rest in the QGP [15,17,48], where H_{int} denotes the coupling Hamiltonian and $|i\rangle$, $|f\rangle$, and $|m\rangle$ the initial, final, and intermediate states, and the box-normalization convention was used. In the present work, the heavy quarkonium transport in the QGP is simulated with Boltzmann equation that embodies the Lorentz-invariant transition amplitudes for the chemical reactions; therefore, the above amplitudes T_{fi} with box normalization needs to be converted into the relativistically normalized (Lorentz-invariant) form $\mathcal{M}$ via [52,53]

$$|\mathcal{M}|^2 = |T_{fi}|^2 \frac{1}{(2\pi)^3 \delta^3(\vec{p}_i - \vec{p}_f) V} \prod_i (2E_i V) \prod_f (2E_f V), \quad (3)$$

where V is the volume used in the box normalization.

For the ground state charmonium J/ψ ($|nlm\rangle = |100\rangle$) under consideration, the Lorentz-invariant amplitude

squared (with the degeneracies of incident gluon and outgoing $Q\bar{Q}$ octet summed over) for the LO reaction ($\Psi + g \leftrightarrow Q + \bar{Q}$) as converted from T_{fi}^{LO} [48] reads

$$\begin{aligned} \sum |\mathcal{M}^{\text{LO}}|^2 &= d_g \frac{g_s^2 \pi}{9} \omega_{\vec{k}} \left[\int r^3 dr j_1(p_{\text{rel}} r) R_{10}(r) \right]^2 \\ &\times (2E_\Psi)(2\omega_{\vec{k}})(2E_Q)(2E_{\bar{Q}}), \end{aligned} \quad (4)$$

where the gluon degeneracy is $d_g = 2 \times 8 = 16$, the incident gluon energy $\omega_{\vec{k}}$, and the relative momentum between Q and $\bar{Q}$ in the color octet $p_{\text{rel}} = |\vec{p}_{\text{rel}}|$. The term in the brackets in Eq. (4) represents the transition matrix element between the bound state and unbound $Q\bar{Q}$ pair, in which j_1 is spherical Bessel function of the first order and $R_{10}(r)$ is the radial wave function of J/ψ computed by solving the Schrödinger equation with a temperature-dependent screening potential [48,54].

The same quantity (again with the degeneracies of incident and outgoing gluons and outgoing $Q\bar{Q}$ octet summed over) for the NLO reaction involving gluons ($\Psi + g \leftrightarrow Q + \bar{Q} + g$) as converted from $T_{fi}^{\text{NLO,g}}$ [17] is

$$\begin{aligned} \sum |\mathcal{M}^{\text{NLO,g}}|^2 &= d_g \frac{g_s^4 \pi}{\omega_{\vec{k}} \omega_{\vec{k}} p_{\text{rel}}^2} \left[\int r^3 dr j_1(p_{\text{rel}} r) R_{10}(r) \right]^2 \\ &\times \left[\frac{\omega_{\vec{k}} - \omega_{\vec{k}}}{\omega_{(\vec{k}-\vec{k})}^2 - (\omega_{\vec{k}} - \omega_{\vec{k}})^2} \right]^2 g(\vec{k}, \vec{p}_{\text{rel}}, \vec{k}) \\ &\times (2E_\Psi)(2\omega_{\vec{k}})(2E_Q)(2E_{\bar{Q}})(2\omega_{\vec{k}}), \end{aligned} \quad (5)$$

where $\omega_{\vec{k}}$ and $\omega_{(\vec{k}-\vec{k})}$ are energies of the outgoing and the exchanged gluons, respectively, and $g(\vec{k}, \vec{p}_{\text{rel}}, \vec{k})$ is a polynomial function of three momenta arising from summing over gluon polarizations (see Ref. [17] for details). Similarly, the Lorentz-invariant amplitude squared (with the degeneracies of incident and outgoing light quarks/antiquarks and outgoing $Q\bar{Q}$ octet summed over) for the NLO reaction involving light quarks/antiquarks ($\Psi + q/\bar{q} \leftrightarrow Q + \bar{Q} + q/\bar{q}$) is given by

$$\begin{aligned} \sum |\mathcal{M}^{\text{NLO,q}}|^2 &= d_q \frac{4g_s^4 \pi}{9E_{\vec{k}} E_{\vec{k}} p_{\text{rel}}^2} \left[\int r^3 dr j_1(p_{\text{rel}} r) R_{10}(r) \right]^2 \\ &\times \left[\frac{E_{\vec{k}} - E_{\vec{k}}}{\omega_{(\vec{k}-\vec{k})}^2 - (E_{\vec{k}} - E_{\vec{k}})^2} \right]^2 f(\vec{k}, \vec{p}_{\text{rel}}, \vec{k}) \\ &\times (2E_\Psi)(2E_{\vec{k}})(2E_Q)(2E_{\bar{Q}})(2E_{\vec{k}}), \end{aligned} \quad (6)$$

where $d_q = 2 \times 2 \times 3 \times 3 = 36$, $E_{\vec{k}}$ and $E_{\vec{k}}$ are energies of incident and outgoing light quarks/antiquarks, and the polynomial $f(\vec{k}, \vec{p}_{\text{rel}}, \vec{k})$ comes from summation over light quark spins (see Ref. [17] for details).

Although what we have computed are the amplitudes for the dissociation processes [17,48], the amplitudes for the

inverse regeneration reactions remain the same as guaranteed by the time reversal symmetry (detailed balance principle). We also note that, in terms of the power counting of the effective field theory [16,50], the LO reaction occurs at the order of $O(g_s r)$, while the NLO reactions are at the order of $O(g_s^2 r)$ [17]. Apart from the dissociation and regeneration reactions, the quantum transitions between different quarkonium eigenstates, e.g., $J/\psi + g \leftrightarrow \psi(2S) + g$, have also been computed, which, however, appear at higher order of $O(g_s^2 r^2)$ [involving the vertex of V_{SO} , Eq. (1), twice] and give significantly smaller rates than the dissociation/regeneration processes [17]. We, therefore, neglect these higher-order transition processes in the present work.

III. SEMICLASSICAL QUARKONIUM TRANSPORT WITH THE BOLTZMANN EQUATION

A. Heavy quarkonium equilibrium limit

In this work, we consider a finite number of single Q and $\bar{Q}$ pairs and one species of quarkonium (ground state J/ψ) that simultaneously transport in a static and homogeneous QGP box. We simulate the dissociation and regeneration reactions as discussed in the previous section and examine the equilibration for the bound state Ψ in the QGP. Should the system be given sufficiently long time to evolve, one expects relative chemical equilibrium to be reached between open $Q\bar{Q}$ and the bound state Ψ , which is dictated by the balance equation in the statistical hadronization model [7–9],

$$N_{Q\bar{Q}} = N_Q^{\text{open}} + N_\Psi. \quad (7)$$

Equation (7) expresses the “balanced” partition of heavy quarks between open $Q\bar{Q}$ and the bound state quarkonium Ψ in the equilibrium limit, under the constraint of heavy flavor number conservation. For a QGP box of fixed volume V and homogeneous temperature T that is much lower than the heavy quark mass,

$$\begin{aligned} N_Q^{\text{open}} &= d_Q \gamma_Q V \int \frac{d^3 p_Q}{(2\pi)^3} e^{-E_Q(\vec{p}_Q)/T} \\ &= d_Q \gamma_Q V \frac{m_Q^2 T}{2\pi^2} K_2\left(\frac{m_Q}{T}\right), \end{aligned} \quad (8)$$

and similarly,

$$N_\Psi = d_\Psi \gamma_Q^2 V \frac{m_\Psi^2 T}{2\pi^2} K_2\left(\frac{m_\Psi}{T}\right), \quad (9)$$

where d_Q and d_Ψ are the degeneracies of single Q and the bound state Ψ , respectively, and the relativistic dispersion relation $E = \sqrt{m^2 + \vec{p}^2}$ has been used to obtain K_2 , the modified Bessel function of the second kind. The heavy

quark fugacity factor γ_Q is introduced in Eqs. (8) and (9) to characterize the deviation of a realistic number of $Q\bar{Q}$ pairs in the system from the absolute chemical equilibrium limit at the given temperature [7–9], which should be self-consistently determined from Eq. (7).

Throughout the work, we fix the number of $Q\bar{Q}$ pairs at $N_{Q\bar{Q}} = 10$, which resembles the realistic situation of $c\bar{c}$ in central Pb-Pb collisions at the LHC energy [28]. As shown by the horizontal dashed lines in Figs. 3 and 5 in Sec. IV, the computed equilibrium limit (with temperature-dependent c quark and J/ψ masses [17]) of the quarkonium yield increases as temperature decreases; that is, $Q\bar{Q}$'s tend to be existing in the form of bound states (with lower energies) at lower temperatures. To compare with pertinent existing studies in literature that also employed semiclassical approaches, but obtained nonrelativistic equilibrium limit [32,36,47], we have also computed such equilibrium limits with $E = m + \frac{\vec{p}^2}{2m}$ in Eqs. (8) and (9).

B. Boltzmann equation for quarkonium evolution

The single-particle phase-space distribution function for single Q ($\bar{Q}$) or quarkonium Ψ reads

$$f_{Q,\bar{Q},\Psi}(\vec{x}, \vec{p}, t) = \frac{dN_{Q,\bar{Q},\Psi}(\vec{x}, \vec{p}, t)}{\frac{d^3 x d^3 p}{(2\pi)^3}}, \quad (10)$$

where the heavy quark fugacity factor and degeneracies have been implicitly incorporated. The $2 \leftrightarrow 2$ and $2 \leftrightarrow 3$ reactions elaborated on in Sec. II are simulated by the Boltzmann equation that keeps track of the time evolution of the quarkonium distribution function

$$\begin{aligned} \frac{d}{dt} f_\Psi(\vec{x}, \vec{p}, t) &= \left(\frac{\partial}{\partial t} + \frac{\partial \vec{x}}{\partial t} \cdot \nabla_{\vec{x}} \right) f_\Psi(\vec{x}, \vec{p}, t) \\ &= C_{22}(\Psi + g \leftrightarrow Q + \bar{Q}) \\ &\quad + C_{23}(\Psi + p \leftrightarrow Q + \bar{Q} + p). \end{aligned} \quad (11)$$

Labeling the momenta involved in the LO process as $\Psi(\vec{p})$, $g(\vec{p}_2)$, $Q(\vec{p}_3)$, $\bar{Q}(\vec{p}_4)$ in the static QGP global frame, the $2 \leftrightarrow 2$ collision term in Eq. (11), in terms of the invariant amplitude $\mathcal{M}^{\text{LO}}$ in Eq. (4), reads

$$\begin{aligned} C_{22} &= C_{22}[\text{gain}] - C_{22}[\text{loss}] \\ &= \frac{1}{2E_\Psi(\vec{p})} \int \frac{d^3 p_2}{2E_g(2\pi)^3} \frac{d^3 p_3}{2E_Q(2\pi)^3} \frac{d^3 p_4}{2E_{\bar{Q}}(2\pi)^3} \\ &\quad \times \sum |\mathcal{M}^{\text{LO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_3 - p_4) \\ &\quad \times \left[\frac{d_\Psi}{d_Q d_{\bar{Q}}} f_Q(\vec{x}, \vec{p}_3, t) f_{\bar{Q}}(\vec{x}, \vec{p}_4, t) (1 + f_g(\vec{x}, \vec{p}_2, t)) \right. \\ &\quad \left. - f_\Psi(\vec{x}, \vec{p}, t) f_g(\vec{x}, \vec{p}_2, t) \right]. \end{aligned} \quad (12)$$

Denoting the pertinent momenta $\Psi(\vec{p})$, $p(\vec{p}_2)$, $Q(\vec{p}_3)$, $\bar{Q}(\vec{p}_4)$, $p(\vec{p}_5)$ again in the QGP global frame and using the amplitudes $\mathcal{M}^{\text{NLO}}$ in Eqs. (5) and (6), the $2 \leftrightarrow 3$ collision term in Eq. (11) can be similarly written as

$$\begin{aligned}
 C_{23} &= C_{23}[\text{gain}] - C_{23}[\text{loss}] \\
 &= \frac{1}{2E_\Psi(\vec{p})} \int \frac{d^3 p_2}{2E_p(\vec{p}_2)(2\pi)^3} \frac{d^3 p_3}{2E_Q(\vec{p}_3)(2\pi)^3} \frac{d^3 p_4}{2E_{\bar{Q}}(\vec{p}_4)(2\pi)^3} \frac{d^3 p_5}{2E_p(\vec{p}_5)(2\pi)^3} \sum |\mathcal{M}^{\text{NLO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_3 - p_4 - p_5) \\
 &\quad \times \left[\frac{d\Psi}{d_Q d_{\bar{Q}}} f_Q(\vec{x}, \vec{p}_3, t) f_{\bar{Q}}(\vec{x}, \vec{p}_4, t) f_p(\vec{x}, \vec{p}_5, t) (1 \pm f_p(\vec{x}, \vec{p}_2, t)) \right. \\
 &\quad \left. - f_\Psi(\vec{x}, \vec{p}, t) f_p(\vec{x}, \vec{p}_2, t) (1 \pm f_p(\vec{x}, \vec{p}_5, t)) \right]. \tag{13}
 \end{aligned}$$

In Eqs. (12) and (13), the Bose/Fermi distribution has been used for gluons/light quarks and the Bose enhancement/Pauli blocking taken into account for final state gluons/light quarks with effective thermal parton masses [17] [the heavier thermal gluon mass than the light quark one makes the Bose-Einstein (B-E) curves lower than the Fermi-Dirac (F-D) ones, as shown in Fig. 1]. Since the amplitudes in Eqs. (4)–(6) are expressed in terms of the Ψ rest frame

variables, $|\mathcal{M}^{\text{LO}}|^2$ and $|\mathcal{M}^{\text{NLO}}|^2$ in Eqs. (12) and (13) should be evaluated by boosting the QGP frame momenta and energies to the rest frame of Ψ .

In the limit when heavy quarks are fully thermalized, the above Boltzmann equation can be reduced to the rate equation for the phase-space distribution of Ψ . To derive this, one notes that the dissociation rate at LO has already been implied in Eq. (12),

$$\Gamma^{\text{LO}}(p, T(\vec{x})) = \frac{1}{2E_\Psi(\vec{p})} \int \frac{d^3 p_2}{2E_g(\vec{p}_2)(2\pi)^3} \frac{d^3 p_3}{2E_Q(\vec{p}_3)(2\pi)^3} \frac{d^3 p_4}{2E_{\bar{Q}}(\vec{p}_4)(2\pi)^3} \sum |\mathcal{M}^{\text{LO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_3 - p_4) f_g(\vec{x}, \vec{p}_2, t). \tag{14}$$

On the other hand, for equilibrium phase distributions f_Q^{eq} and $f_{\bar{Q}}^{\text{eq}}$ for the single heavy quarks, one has

$$\begin{aligned}
 \frac{d\Psi}{d_Q d_{\bar{Q}}} f_Q^{\text{eq}}(\vec{p}_3) f_{\bar{Q}}^{\text{eq}}(\vec{p}_4) (1 + f_g(\vec{p}_2)) &= d_\Psi \gamma_Q e^{-E_Q(\vec{p}_3)/T} \gamma_{\bar{Q}} e^{-E_{\bar{Q}}(\vec{p}_4)/T} \left(1 + \frac{1}{e^{E_g(\vec{p}_2)/T} - 1} \right) \\
 &= d_\Psi \gamma_Q^2 e^{(-E_Q(\vec{p}_3) - E_{\bar{Q}}(\vec{p}_4) + E_g(\vec{p}_2))/T} \frac{1}{e^{E_g(\vec{p}_2)/T} - 1} \\
 &= d_\Psi \gamma_Q^2 e^{-E_\Psi(\vec{p})/T} \frac{1}{e^{E_g(\vec{p}_2)/T} - 1} \\
 &= f_\Psi^{\text{eq}}(\vec{p}) f_g(\vec{p}_2), \tag{15}
 \end{aligned}$$

where the $\vec{x}$ dependence has been omitted, and f_Ψ^{eq} is the equilibrium phase-space distribution for the bound state Ψ . Combining (14) and (15), Eq. (12) can be simplified to the rate equation for the LO reaction

$$\frac{d}{dt} f_\Psi(\vec{x}, \vec{p}, t) = -\Gamma^{\text{LO}}(p, T(\vec{x})) [f_\Psi(\vec{x}, \vec{p}, t) - f_\Psi^{\text{eq}}(\vec{x}, \vec{p})]. \tag{16}$$

Similarly, combining the NLO dissociation rate embodied in Eq. (13),

$$\begin{aligned}
 \Gamma^{\text{NLO,g/q}}(p, T(\vec{x})) &= \frac{1}{2E_\Psi(\vec{p})} \int \frac{d^3 p_2}{2E_p(\vec{p}_2)(2\pi)^3} \frac{d^3 p_3}{2E_Q(\vec{p}_3)(2\pi)^3} \frac{d^3 p_4}{2E_{\bar{Q}}(\vec{p}_4)(2\pi)^3} \frac{d^3 p_5}{2E_p(\vec{p}_5)(2\pi)^3} \sum |\mathcal{M}^{\text{NLO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_3 - p_4 - p_5) \\
 &\quad \times f_p(\vec{x}, \vec{p}_2, t) (1 \pm f_p(\vec{x}, \vec{p}_5, t)), \tag{17}
 \end{aligned}$$

and

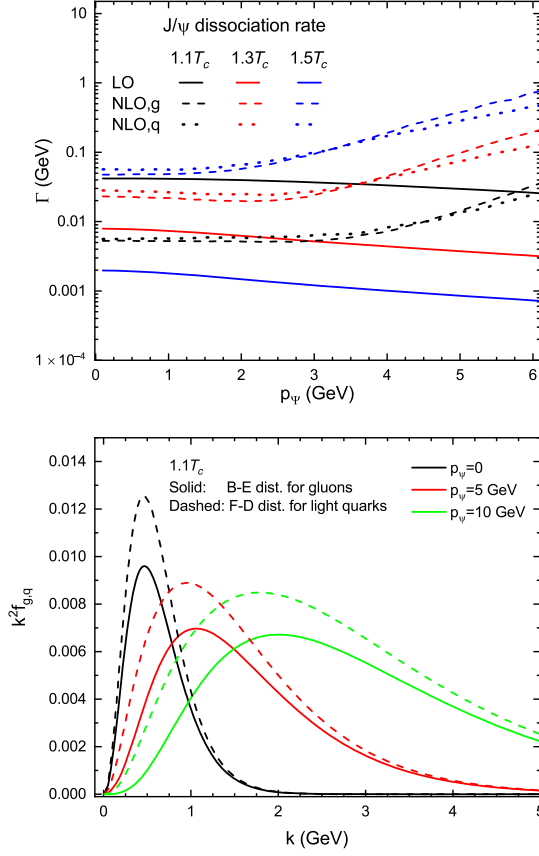


FIG. 1. Upper: dissociation rates for J/ψ with finite momentum at different temperatures; contributions from LO (solid), gluon-induced NLO (dashed), and light quark-induced NLO (dotted) processes are displayed separately. Lower: thermal distributions of incident partons seen by the heavy quarkonium as function of parton momentum, for varying J/ψ momenta at $1.1T_c$.

$$\begin{aligned}
 & \frac{d\Psi}{dQ d\bar{Q}} f_Q^{\text{eq}}(\vec{p}_3) f_{\bar{Q}}^{\text{eq}}(\vec{p}_4) f_p(\vec{p}_5) (1 \pm f_p(\vec{p}_2)) \\
 &= d\Psi \gamma_Q^2 e^{-(E_Q(\vec{p}_3) + E_{\bar{Q}}(\vec{p}_4) - E_p(\vec{p}_2))/T} \\
 &\times \frac{1}{e^{E_p(\vec{p}_5)/T} \mp 1} \frac{1}{e^{E_p(\vec{p}_2)/T} \mp 1} \\
 &= d\Psi \gamma_Q^2 e^{-(E_p(\vec{p}) - E_g(\vec{p}_5))/T} \frac{1}{e^{E_p(\vec{p}_5)/T} \mp 1} \frac{1}{e^{E_p(\vec{p}_2)/T} \mp 1} \\
 &= f_{\Psi}^{\text{eq}}(\vec{p}) f_p(\vec{p}_2) (1 \pm f_p(\vec{p}_5)), \quad (18)
 \end{aligned}$$

Eq. (13) is reduced to the rate equation for the NLO reaction

$$\frac{d}{dt} f_{\Psi}(\vec{x}, \vec{p}, t) = -\Gamma^{\text{NLO,g/q}}(p, T(\vec{x})) [f_{\Psi}(\vec{x}, \vec{p}, t) - f_{\Psi}^{\text{eq}}(\vec{x}, \vec{p})]. \quad (19)$$

Furthermore, if the dissociation rates involved in Eqs. (16) and (19) are replaced by the momentum-averaged ones, the phase-space distributions can be integrated to produce the rate equation for the yield of Ψ ,

$$\frac{d}{dt} N_{\Psi}(t) = -\Gamma(\langle p \rangle, T) [N_{\Psi}(t) - N_{\Psi}^{\text{eq}}], \quad (20)$$

which has been widely used for describing the heavy quarkonium transport in literature [23,55]. In Eq. (20), the equilibrium yield N_{Ψ}^{eq} of Ψ now acts as a transport coefficient associated with regeneration. The above derivation of the rate equations suggests that heavy quarkonium equilibration through dissociation and regeneration dynamics relies on the kinetic thermalization of single Q and $\bar{Q}$ in advance.

C. Dissociation of quarkonium

We first evaluate the dissociation rates as defined in Eqs. (14) and (17) for a heavy quarkonium moving in QGP, which will be used for the numerical simulations in Sec. IV. By solving the Schrödinger equation with temperature-dependent heavy quark potential, the dissociation temperature for the ground state charmonium J/ψ has been determined to be at about $1.6T_c$ (T_c being the pseudocritical temperature) [17]. The dissociation temperature is also considered to be the onset point for the bound state regeneration. Therefore, in this work, we perform the heavy quarkonium transport simulations in a static QGP at three constant temperatures: $T = 1.1T_c$, $1.3T_c$, and $1.5T_c$ for the purpose of illustration.

The numerical results for the dissociation rates $\Gamma(p, T)$ as function of J/ψ momentum at different temperatures are displayed in the upper panel of Fig. 1. At the lowest temperature $1.1T_c$, the LO dissociation rates dominate over the NLO counterparts in the low momentum region. However, as temperature increases, the LO rates start to lose steam, while the NLO rates keep growing and take over. As for the momentum dependence of these rates, the LO rates monotonously decrease with increasing momentum, but the NLO rates generally increase toward high momenta. The similar momentum dependence for the Ψ 's dissociation rates was also found in [35,37]. To understand these behaviors, we examine the thermal parton phase-space distribution function from the perspective of the rest frame of the Ψ . The thermal distribution of gluons or light quarks seen by the Ψ reads $k^2 / (e^{\gamma(E(\vec{k}) + \vec{k} \cdot \vec{v})/T} \mp 1)$, with k being the thermal parton's momentum and γ the Lorentz factor associated with the quarkonium's moving velocity v in the QGP global frame. As shown in the lower panel of Fig. 1, for increasing momentum of the Ψ , the parton distributions shift toward higher momentum. Therefore, the convolution of LO cross section with the gluon distribution, i.e., LO dissociation rate, reduces with Ψ momentum increasing, since the LO cross section for a quarkonium at rest peaks at relatively low incident gluon energy and falls off toward higher energy [14,48,56]. In contrast, the NLO cross section gradually grows with incident parton energy and finally saturates [17], which makes its overlap with the thermal parton phase-space distributions grow

with the incident parton energy (measured in the Ψ 's rest frame), thereby yielding increasing rates for larger Ψ momentum as seen from the QGP global frame. We also note that the rates arising from the gluon-induced NLO process are slightly smaller at low momenta and become larger toward higher momenta compared to the light quark counterparts.

Taking advantage of the homogeneity of the static QGP box, one needs to only keep track of the Ψ 's momentum distribution $f_\Psi(\vec{p}, t)$ obtained by integrating out the coordinates of the phase-space distribution function. Using the dissociation rates $\Gamma(p, T)$, the iteration scheme for the loss in $f_\Psi(\vec{p}, t)$ can be constructed as

$$\begin{aligned} \frac{d}{dt} f_\Psi(\vec{p}, t) [\text{loss}] &= - \int \frac{d^3x}{(2\pi)^3} \Gamma(p, T) f_\Psi(\vec{x}, \vec{p}, t) \\ &= -\Gamma(p, T) f_\Psi(\vec{p}, t). \end{aligned} \quad (21)$$

$$\begin{aligned} \frac{d}{dt} f_\Psi(\vec{p}, t) [\text{gain}, 2 \leftrightarrow 2] &= \int \frac{d^3x}{(2\pi)^3} C_{22} [\text{gain}] \\ &= \frac{d_\Psi}{d_Q d_{\bar{Q}}} \frac{1}{2E_\Psi(\vec{p})} \sum_{n_Q=1}^{N_Q} \sum_{n_{\bar{Q}}=1}^{N_{\bar{Q}}} \int \frac{d^3p_2}{2E_g(2\pi)^3} \frac{1}{2E_Q} \frac{1}{2E_{\bar{Q}}} \sum |\mathcal{M}^{\text{LO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_{n_Q} - p_{n_{\bar{Q}}}) \\ &\quad \times \int \frac{d^3x}{(2\pi)^3} \delta^3(\vec{x} - \vec{x}_{n_Q}(t)) \delta^3(\vec{x} - \vec{x}_{n_{\bar{Q}}}(t)) (1 + f_g(\vec{x}, \vec{p}_2, t)) \\ &= \frac{d_\Psi}{d_Q d_{\bar{Q}}} \frac{1}{2E_\Psi(\vec{p})} \sum_{n_Q=1}^{N_Q} \sum_{n_{\bar{Q}}=1}^{N_{\bar{Q}}} \frac{1}{2E_g} \frac{1}{2E_Q} \frac{1}{2E_{\bar{Q}}} \sum |\mathcal{M}^{\text{LO}}|^2 (2\pi) \delta(E_\Psi(\vec{p}) + E_g(\vec{p}_2) - E_Q(\vec{p}_{n_Q}) - E_{\bar{Q}}(\vec{p}_{n_{\bar{Q}}})) \\ &\quad \times \frac{1}{(2\pi)^3} \delta^3(\vec{x}_{n_Q}(t) - \vec{x}_{n_{\bar{Q}}}(t)) (1 + f_g(\vec{x}, \vec{p}_2, t)), \end{aligned} \quad (23)$$

where in the last step, $\vec{p}_2 = -\vec{p} + \vec{p}_{n_Q} + \vec{p}_{n_{\bar{Q}}}$, and the gluon position is taken to be $\vec{x} = (\vec{x}_{n_Q}(t) + \vec{x}_{n_{\bar{Q}}}(t))/2$. In practice, the δ function involving the spatial separation between Q and $\bar{Q}$ is smeared by a Gaussian function [32]

$$\delta^3(\vec{x}_{n_Q}(t) - \vec{x}_{n_{\bar{Q}}}(t)) \approx \frac{\exp[-(\vec{x}_{n_Q}(t) - \vec{x}_{n_{\bar{Q}}}(t))^2 / (2\sigma^2)]}{(2\pi\sigma^2)^{3/2}}. \quad (24)$$

It has been numerically checked that the choice of the spatial scale σ in a relatively large range, e.g., $\sigma \in [0.15 \text{ fm}, 0.75 \text{ fm}]$, does not affect the numerical results. This is because, when a smaller (larger) σ is employed, the effective number of $Q\bar{Q}$ pairs that are encompassed and participate in recombination is reduced (increased), which is, however, balanced by the larger (smaller) recombination probability arising from the

D. Recombination from single Q and $\bar{Q}$

We move on to discuss the implementation of the gain terms of Boltzmann equation that corresponds to the regeneration from diffusing Q and $\bar{Q}$. Generally the phase-space distributions for single Q and $\bar{Q}$ can be represented via the test-particle method [32],

$$\begin{aligned} f_Q(t, \vec{x}, \vec{p}) &= \sum_{n_Q=1}^{N_Q} (2\pi)^3 \delta^3(\vec{x} - \vec{x}_{n_Q}(t)) \delta^3(\vec{p} - \vec{p}_{n_Q}(t)), \\ f_{\bar{Q}}(t, \vec{x}, \vec{p}) &= \sum_{n_{\bar{Q}}=1}^{N_{\bar{Q}}} (2\pi)^3 \delta^3(\vec{x} - \vec{x}_{n_{\bar{Q}}}(t)) \delta^3(\vec{p} - \vec{p}_{n_{\bar{Q}}}(t)). \end{aligned} \quad (22)$$

First, the gain term for the $2 \leftrightarrow 2$ process can be cast into a more tractable form in terms of the single Q and $\bar{Q}$ test particles, by substituting Eq. (22) into Eq. (12) and integrating over the coordinate,

enhanced (reduced) strength of the sharper (wider) Gaussian peak. As a result, the final results are rather robust against the variation of σ , when averaged over a large number of events in the simulation. Practically, since σ characterizes the recombination range in coordinate space, one can choose σ to be equal to the Bohr radius of bound state Ψ [32,36]. Finally, for relativistic Q and $\bar{Q}$, the δ function ensuring energy conservation in Eq. (23), $f(p_z) = \sqrt{m_\Psi^2 + \vec{p}_T^2 + p_z^2} + \sqrt{m_g^2 + \vec{p}_{2,T}^2 + p_{2,z}^2} - \sqrt{m_Q^2 + \vec{p}_{n_Q}^2} - \sqrt{m_{\bar{Q}}^2 + \vec{p}_{n_{\bar{Q}}}^2} = 0$, can be eliminated via

$$\left. \frac{dN}{p_T dp_T d\phi_p dp_z} \right|_{f(p_z)=0} \propto \frac{\int dp_z \delta(f(p_z))}{\Delta p_z}, \quad (25)$$

which becomes accurate when Δp_z is small enough.

Next by plugging Eq. (22) into Eq. (13) and integrating out the coordinates, the gain term due to the $2 \leftrightarrow 3$ process can be similarly handled,

$$\begin{aligned}
\frac{d}{dt} f_\Psi(\vec{p}, t) [\text{gain}, 2 \leftrightarrow 3] &= \int \frac{d^3 x}{(2\pi)^3} C_{23} [\text{gain}] \\
&= \frac{d_\Psi}{d_Q d_{\bar{Q}}} \frac{1}{2E_\Psi(\vec{p})} \sum_{n_Q=1}^{N_Q} \sum_{n_{\bar{Q}}=1}^{N_{\bar{Q}}} \int \frac{d^3 p_2}{2E_p(\vec{p}_2)(2\pi)^3} \frac{1}{2E_Q} \frac{1}{2E_{\bar{Q}}} \frac{d^3 p_5}{2E_p(\vec{p}_5)(2\pi)^3} \\
&\quad \times \sum |\mathcal{M}^{\text{NLO}}|^2 (2\pi)^4 \delta^4(p + p_2 - p_{n_Q} - p_{n_{\bar{Q}}} - p_5) \\
&\quad \times \frac{1}{(2\pi)^3} \delta^3(\vec{x}_{n_Q}(t) - \vec{x}_{n_{\bar{Q}}}(t)) f_p(\vec{x}, \vec{p}_5, t) (1 \pm f_p(\vec{x}, \vec{p}_2, t)) \\
&= \frac{d_\Psi}{d_Q d_{\bar{Q}}} \frac{1}{2E_\Psi(\vec{p})} \sum_{n_Q=1}^{N_Q} \sum_{n_{\bar{Q}}=1}^{N_{\bar{Q}}} \int \frac{p_2^2 d\Omega_{\vec{p}_2}}{2E_p(\vec{p}_2)(2\pi)^3} \frac{1}{2E_Q} \frac{1}{2E_{\bar{Q}}} \frac{1}{2E_p(\vec{p}_5)} \\
&\quad \times \sum |\mathcal{M}^{\text{NLO}}|^2 \frac{2\pi}{|f'(p_2)|} \frac{1}{(2\pi)^3} \delta^3(\vec{x}_{n_Q}(t) - \vec{x}_{n_{\bar{Q}}}(t)) f_p(\vec{x}, \vec{p}_5, t) (1 \pm f_p(\vec{x}, \vec{p}_2, t)), \quad (26)
\end{aligned}$$

where $\vec{p}_5 = \vec{p} + \vec{p}_2 - \vec{p}_{n_Q} - \vec{p}_{n_{\bar{Q}}}$, and $p_2 = |\vec{p}_2|$ is calculated from $f(p_2) = E_\Psi(\vec{p}) + E_p(\vec{p}_2) - E_Q(\vec{p}_{n_Q}) - E_{\bar{Q}}(\vec{p}_{n_{\bar{Q}}}) - E_p(\vec{p}_5) = 0$, leaving only integration over the polar angle of $\vec{p}_2$.

In summary, Eqs. (23) and (26) represent the iteration scheme for the gain (due to the LO and NLO regeneration/recombination reactions) in the Ψ 's momentum distribution $f_\Psi(\vec{p}, t)$, which, in combination with the iteration scheme constructed for the loss in $f_\Psi(\vec{p}, t)$ [cf. Eq. (21)], constitute the core method underlying our simulation for the Ψ 's equilibration. We also note that the regeneration dynamics of heavy quarkonium Ψ in the present approach is driven by the realistic quantum-mechanical scattering amplitudes involving the participant Q , $\bar{Q}$ and light partons, in which the bound state wave function has been explicitly incorporated, cf. Eqs. (4)–(6). This is in marked contrast to a recent study [47] on the same topic based on measuring the relative energy of the Q and $\bar{Q}$ pairs. For the latter, an attractive force term arising from the real part of the complex heavy quark potential [19] was added on top of the Langevin equation for the Q and $\bar{Q}$'s diffusion. A bound state was then considered to be formed (destroyed) as long as the relative energy between Q and $\bar{Q}$ is negative (positive), which amounts to a purely classical criterion involving no quantum wave function effects. Our method is similar to the one used in [32,36] where the dynamical scattering amplitudes were also employed to describe the transition between bound state and unbound heavy quark pairs. However, in these latter works, the simulation was performed in a full Monte Carlo way such that the Ψ 's were also treated as test particles by sampling the differential rates and the equilibrium limit obtained was nonrelativistic [32,36].

IV. NUMERICAL SIMULATIONS AND RESULTS

As specified before, our simulations for quarkonium equilibration are performed in a static QGP box of fixed volume $L^3 = (10 \text{ fm})^3$ and homogeneous temperature T . The initial positions of heavy quarks are uniformly sampled and the periodic boundary condition is imposed for test particles Q and $\bar{Q}$ in a finite size box. Because of the latter, when performing the recombination of Q and $\bar{Q}$, the relative distance within that pair is counted by

$$r^i = \min \{ |x_Q^i - x_{\bar{Q}}^i|, L - |x_Q^i - x_{\bar{Q}}^i| \}, \quad i = 1, 2, 3, \quad (27)$$

with $x_{Q/\bar{Q}}^i$ being the real-time position of $Q/\bar{Q}$ in the i th direction. Equation (27) is known as the minimum image convention and is widely adopted in literature [42].

A. Thermalized Q and $\bar{Q}$

We first perform a test simulation for heavy quarkonium chemical equilibration in the extreme case of full thermalization of single heavy quarks before embarking on more realistic simulation with nonequilibrium (i.e., transported) heavy quarks.

Since the regeneration plays a key role for quarkonium equilibration, let us first quantify the features of pure regeneration through LO and NLO processes via Eqs. (23) and (26), by using ten pairs of c and $\bar{c}$ that are fully thermalized, i.e., $f(\vec{p}_Q) \propto e^{-E_Q(\vec{p}_Q)/T} = e^{-\sqrt{m_Q^2 + \vec{p}_Q^2}/T}$. The time evolution of the yield of purely regenerated Ψ is displayed in the upper panel of Fig. 2 for three temperatures. At a fixed temperature, the regenerated Ψ yield simply keeps growing with time at a constant slope that can be extracted as the absolute regeneration rate (characterizing the absolute

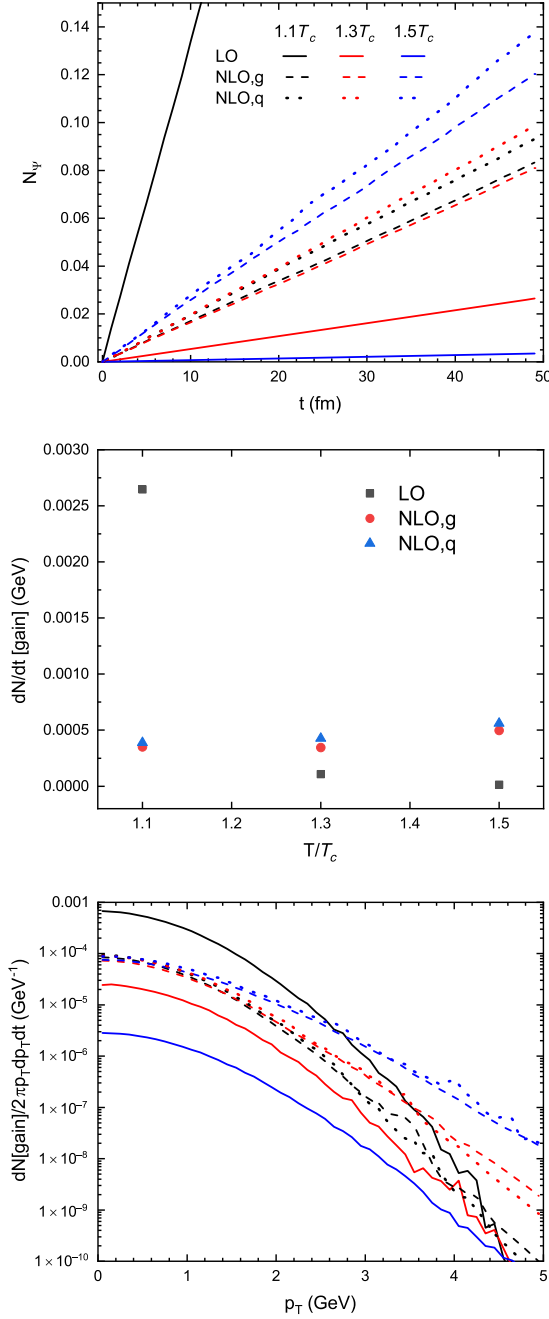


FIG. 2. Upper: the time evolution of J/ψ regenerated from ten pairs of thermalized c and $\bar{c}$ at varying temperatures; contributions from different dynamical processes are displayed separately. Middle: regeneration rates extracted from upper panel. Lower: p_T -differential regeneration rates in the simulations.

increase in the J/ψ number as obtained from regeneration processes within unit time) and is presented in the middle panel of Fig. 2. The LO regeneration rates are pronounced at $1.1T_c$ but decline rapidly toward higher temperatures. In contrast, the NLO regeneration rates show a general increase with T and take over from LO at high temperatures; the light quark-induced NLO regeneration rates are always slightly larger than the gluon-induced one. Since here the Q and $\bar{Q}$'s

are assumed fully thermalized, these behaviors of the regeneration rates can be understood from the gain term of the rate equation for the integrated yield [Eq. (20)]: $dN_\Psi(t)/dt[\text{gain}] = \Gamma(\langle p \rangle, T)N_\Psi^{\text{eq}}$, where the temperature dependence of the dissociation rates (decreasing/increasing with temperature for LO/NLO) as shown in the upper panel of Fig. 1 is strengthened/mitigated by the equilibrium yield N_Ψ^{eq} which reduces toward high temperatures. Furthermore, the p_T -differential regeneration rates are displayed in the lower panel of Fig. 2. As temperature increases, the p_T spectra of both LO and NLO regeneration rates become harder, simply because the momentum distributions of thermalized Q and $\bar{Q}$ participating in recombination are harder. Another observation is that the p_T spectrum of the LO regeneration rates is always softer than that from the NLO process, which is attributed to the softer momentum dependence of the LO dissociation rates than the NLO ones (upper panel of Fig. 1) embodied in the gain term of the (now momentum-dependent) rate equations (16) and (19).

Now we simulate the regeneration and the dissociation simultaneously. The conservation of heavy quarks, i.e., $N_{Q\bar{Q}} = N_Q^{\text{open}} + N_\Psi = 10$, is imposed throughout the evolution. Since the Q and $\bar{Q}$'s participating in recombination are treated as test particles, their numbers are required to be integers. However, as the evolution goes on, the real-time yield of the bound states is not an integer any more and neither is the number of Q and $\bar{Q}$'s. To handle this situation, we envision that there are always $\mathcal{N}_Q = \mathcal{N}_{\bar{Q}} = 10$ and use them to compute the regeneration via Eqs. (23) and (26), but the resulting regenerated bound state yield should be rescaled by $(\mathcal{N}_Q - N_\Psi(t))(\mathcal{N}_{\bar{Q}} - N_\Psi(t))/(\mathcal{N}_Q\mathcal{N}_{\bar{Q}})$, with $N_\Psi(t)$ being the real-time number of Ψ . This rescaling becomes more important when one has a nonzero number of bound states at the initialization time.

We consider two kinds of initial conditions, i.e., initially there is no bound state [$N_\Psi(0) = 0$] and initially there is one bound state [$N_\Psi(0) = 1$]. For the latter case, we set the Ψ initial momentum distribution as being thermalized. The numerical results for the time evolution of the integrated yield of Ψ at three different temperatures are depicted in Fig. 3, where different dynamical processes (LO, NLO induced by gluons, and NLO induced by light quarks/antiquarks) are compared. For both of the two initial conditions, after sufficiently long time evolution, the bound state abundance exhibits clear convergence toward the chemical equilibrium limit, as given by the balance equation (7). We find that the time required for Ψ 's yield to reach equilibrium limit through LO reactions at $1.1T_c$ is shorter compared to that through NLO processes, but at higher temperatures, the LO chemical equilibration becomes much slower. For instance, at $1.3T_c$, when there is no bound state initially, it takes ~ 30 fm for NLO reactions to achieve chemical equilibrium, while the equilibration time for the LO reaction reaches ~ 80 fm. This is in line with the fact that the LO rates (both the

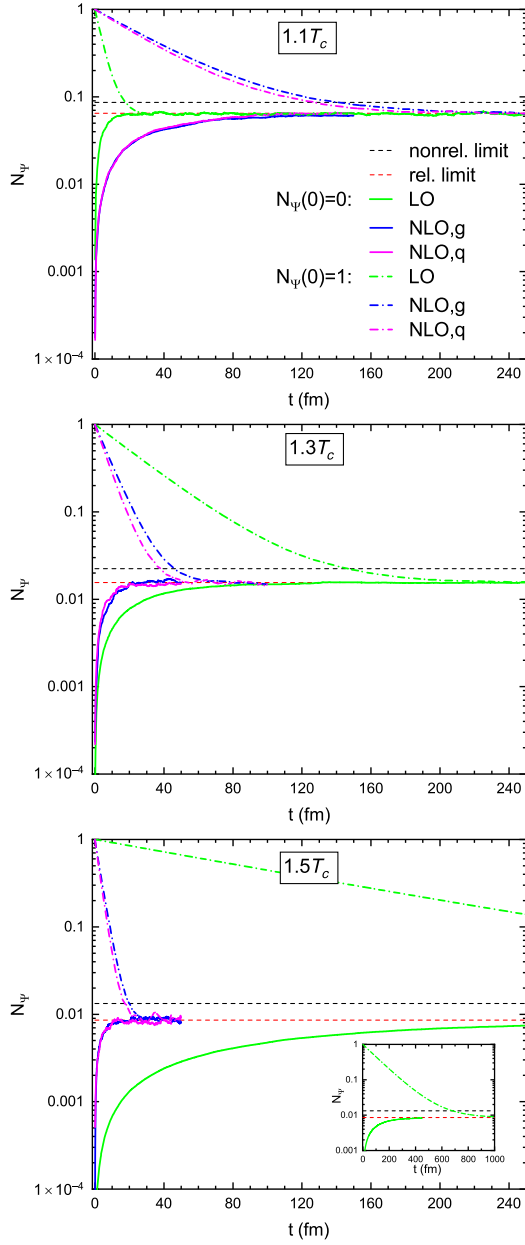


FIG. 3. The time evolution of the J/ψ yield by simulating regeneration and dissociation simultaneously at $1.1T_c$ (top), $1.3T_c$ (middle), and $1.5T_c$ (bottom), where the regeneration is computed from thermalized c and $\bar{c}$. The horizontal black and red dashed lines correspond to the relative chemical equilibrium limits of J/ψ integrated yields computed by the balance equation (7) with nonrelativistic and relativistic dispersion relations, respectively. Different initial conditions and different dynamical processes are shown for comparison.

dissociation and regeneration, as discussed in Secs. III C and III D) are larger than NLO ones at low temperatures, while the latter take over at high temperatures. One also notices that, at all temperatures and for all chemical reactions, when there is one bound state initially [$N_\Psi(0) = 1$], the equilibration is always slowed down

compared to there being no bound state initially [$N_\Psi(0) = 0$], although the momentum distribution of the initial bound state has been assumed to be thermal. For example, still at $1.3T_c$, the equilibration time with the initial condition $N_\Psi(0) = 1$ reaches ~ 60 and ~ 200 fm for the NLO and LO reactions, respectively, which are around 2–2.5 times longer compared to the case with the initial condition $N_\Psi(0) = 0$. All these observations are consistent with the empirical fact that chemical equilibration usually lags behind the kinetic equilibration.

B. Transported Q and $\bar{Q}$

Now, we turn to the simulations of heavy quarkonium equilibration with more realistic nonequilibrium (i.e., transported) single heavy quarks. In heavy-ion collisions, the heavy quarks are produced from the initial hard processes and thus their initial momentum distributions are far from thermalized. Once the QGP forms, the heavy quarks diffuse and thermalize in the medium through rescatterings with thermal partons [2]. The diffusion of heavy quarks can be simulated by the Langevin equations [57]

$$d\vec{x} = \frac{\vec{p}}{E_p} dt, \quad d\vec{p} = -\Gamma(p, T)\vec{p}dt + \sqrt{2dtD(\vec{p} + d\vec{p})}\vec{p}, \quad (28)$$

where $E_p = \sqrt{m^2 + \vec{p}^2}$. For the purpose of illustration, we use a constant (momentum- and temperature-independent) drag coefficient (or thermal relaxation rate), $\Gamma(p, T) = \gamma = 0.1 \text{ fm}^{-1}$. The momentum diffusion coefficient in Eq. (28) is related to the relaxation rate via the Einstein relation, $D(p) = \gamma E_p T$ [57]. The c quark diffusion in the static QGP box is then simulated utilizing the postpoint Langevin scheme [57], with their initial momenta being uniformly distributed in the range $-5 < p_i < 5 \text{ GeV}$, $i = 1, 2, 3$. The time evolution for the c quark p_T and p_z distributions is displayed in Fig. 4 for fixed temperature $1.3T_c$. It takes ~ 30 – 40 fm for these momentum distributions to approach the Boltzmann equilibrium limit, as indicated by the red dashed lines in Fig. 4, which can be regarded as the kinetic equilibration (i.e., thermalization) time for heavy quarks.

Then we perform the simulation of heavy quarkonium equilibration by coupling the bound state dissociation and regeneration dynamics [Eqs. (21), (23), and (26)] with the Langevin diffusion of single heavy quarks [Eq. (28)] in a real-time fashion. The results for the evolution of the bound state yield for different reactions are shown in Fig. 5 at different temperatures. Comparing to the case when heavy quarks are assumed to be fully thermalized from the beginning, as discussed in Sec. IV A, now it generally takes longer time for the quarkonium Ψ to reach chemical equilibrium. For example, at $1.3T_c$, the equilibration time via the NLO reactions now reaches ~ 50 fm with initial

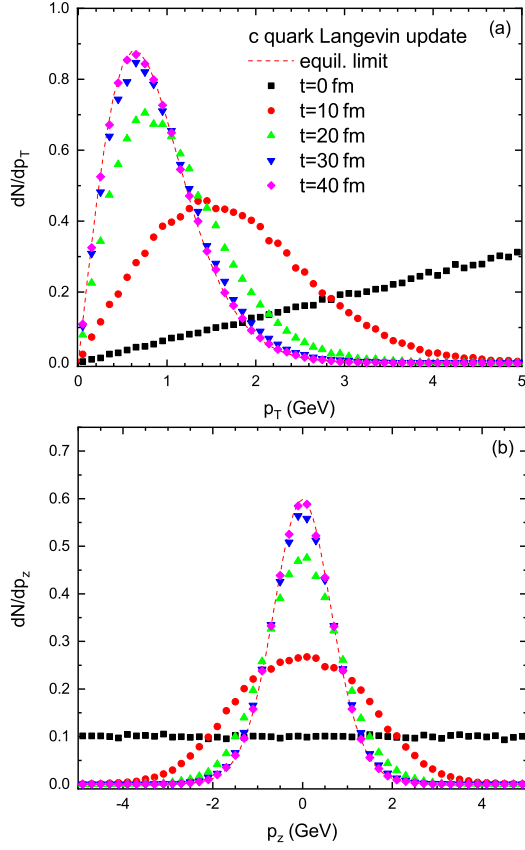


FIG. 4. The evolution of charm quark normalized p_T (a) and p_z (b) distributions through Langevin simulation at $1.3T_c$, by using a constant thermal relaxation rate $\gamma = 0.1 \text{ fm}^{-1}$. The red dashed lines represent the Boltzmann distributions of charm quarks.

condition $N_\Psi(0) = 0$, which reduces to $\sim 20 \text{ fm}$ if heavy quarks are always thermalized (see the middle panel of Fig. 3). This is because the regeneration rates are sensitively dependent upon the degree of the heavy quark thermalization—regeneration is generally delayed for non-thermalized heavy quarks. Consequently, quarkonium equilibration must lag behind the kinetic thermalization of heavy quarks which takes 30–40 fm at $1.3T_c$, as shown in Fig. 4.

We also note that now, at a given temperature, the equilibration times are almost equal for two different initial conditions, in cases where the reaction rates are sufficiently large (e.g., the LO reaction at $1.1T_c$, the NLO reactions at $1.3T_c$ and $1.5T_c$). This is because, in the early stage of the evolution, the regeneration is still inefficient because heavy quarks are far from being thermalized, which is the same for both kinds of initial conditions. However, for $N_\Psi(0) = 1$, the initial reaction dynamics is dominated by dissociation and thus this J/ψ could be quickly dissociated. Only after the initial bound state is mostly gone and the heavy quarks thermalize to a large extent does regeneration proceed efficiently toward the equilibrium limit, making the equilibration time insensitive to the initial conditions. Actually, as

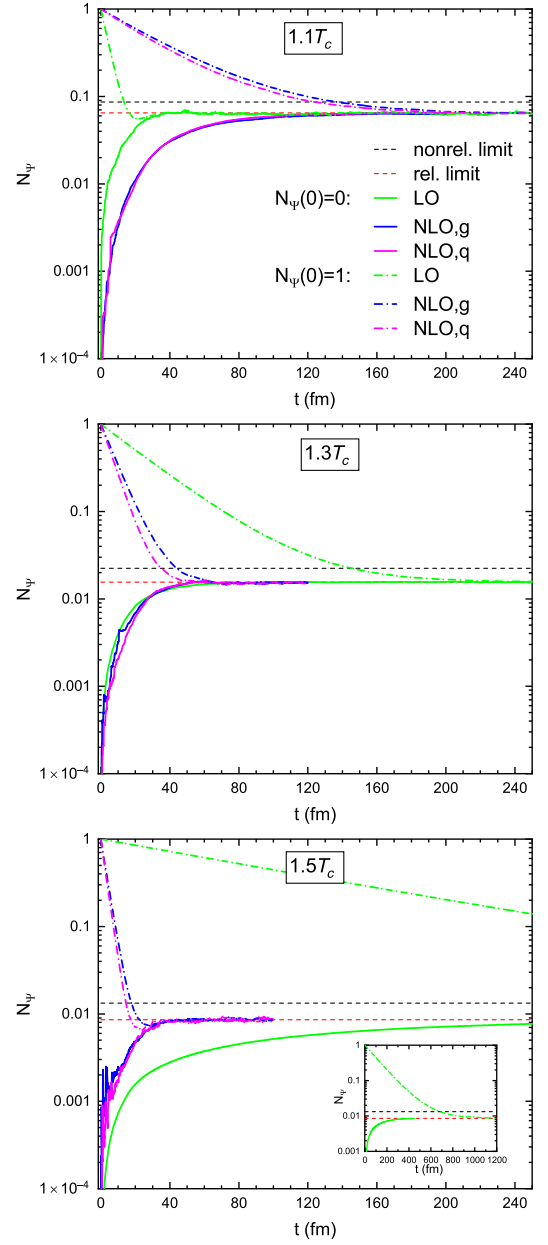


FIG. 5. Similar to Fig. 3, but the transport of the bound state is coupled with the single heavy quark Langevin simulations, i.e., regeneration here is computed from transported c and $\bar{c}$.

manifested in the LO reaction at $1.1T_c$ (dash-dotted green line in upper panel of Fig. 5) and the NLO reaction at $1.5T_c$ (dash-dotted purple/blue line in lower panel of Fig. 5) with $N_\Psi(0) = 1$, the early-time dissociation is so much dominant that the resulting bound state yield can fall below the equilibrium limit. This deficiency relative to the equilibrium yield is then compensated for by the efficient regeneration after the heavy quarks get fully thermalized, so that finally the bound state yield approaches the equilibrium limit.

Finally, the quarkonium p_T and p_z distributions after the relative chemical equilibrium for the quarkonium yields has been reached (Fig. 5) are shown in Fig. 6. These distributions

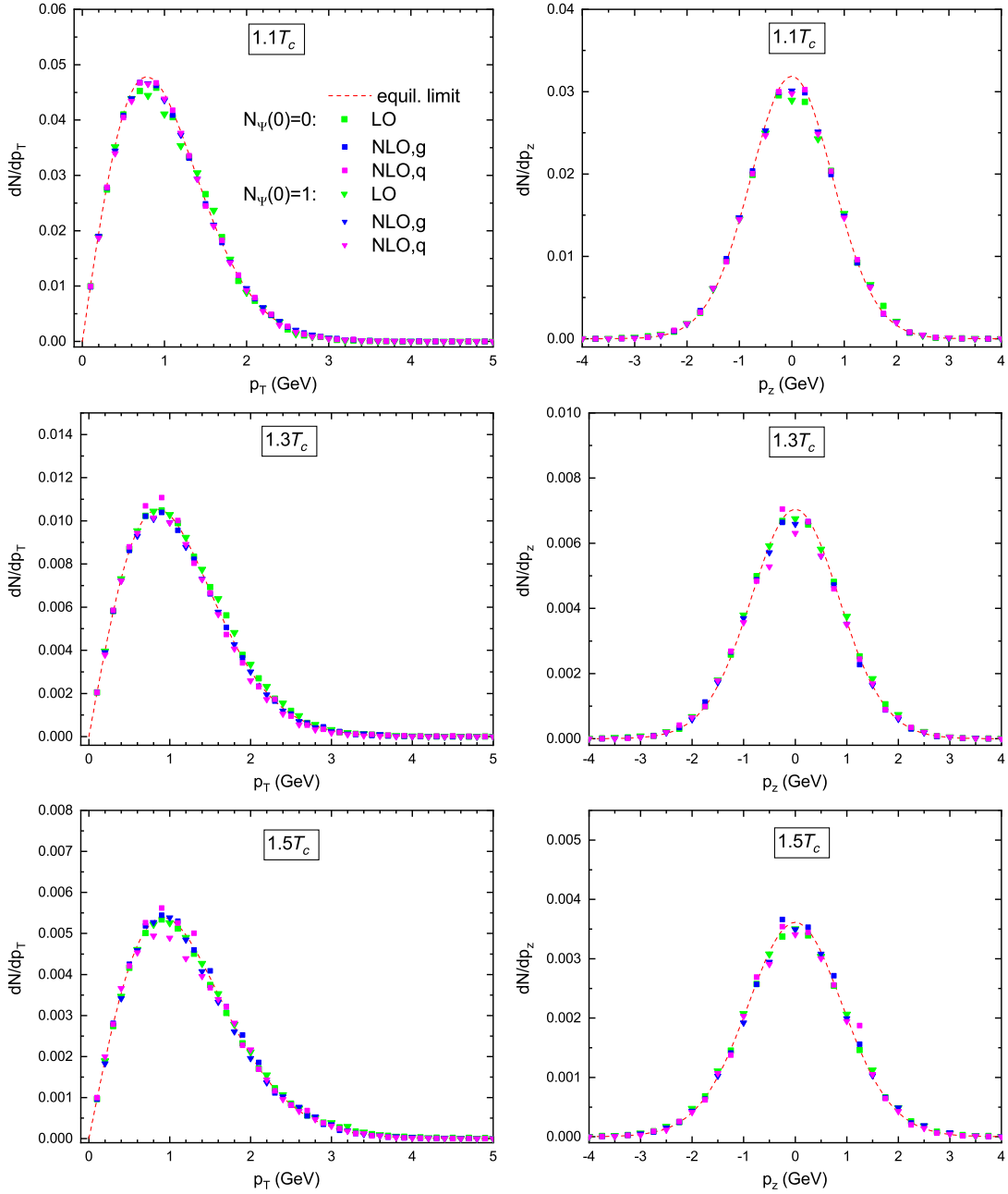


FIG. 6. The (left) p_T and (right) p_z distributions of J/ψ after the relative chemical equilibrium has been reached. The red dashed lines represent the Boltzmann distributions of J/ψ with relativistic dispersion relation at varying temperatures; the norms correspond to the chemical equilibrium values presented in the horizontal red dashed lines in Figs. 3 and 5.

(absolute spectra without artificial shift in norm) turn out to agree well with Boltzmann distributions (red dashed lines) underlying the equilibrium limit in the balance equation (7). This implies, as expected, that kinetic equilibrium for the momentum distributions is already embodied in the (relative) chemical equilibrium for the quarkonium yield.

C. Equilibration with total reaction rates

Having theoretically analyzed and compared the heavy quarkonium equilibration processes for various LO and

NLO reactions, we finally conduct a simulation for the equilibration using the total reaction rates (LO and NLO combined) and transported charm quarks with phenomenologically more relevant yet still constant thermal relaxation rate $\gamma = 0.4 \text{ fm}^{-1}$ [58,59], in order to make a quantitatively more realistic estimate for the heavy quarkonium equilibration times. For this, the initial momentum distributions for the single charm quark and also for the bound state J/ψ [for the initial condition $N_\psi(0) = 1$] used in Sec. IV B are also replaced with the more realistic ones

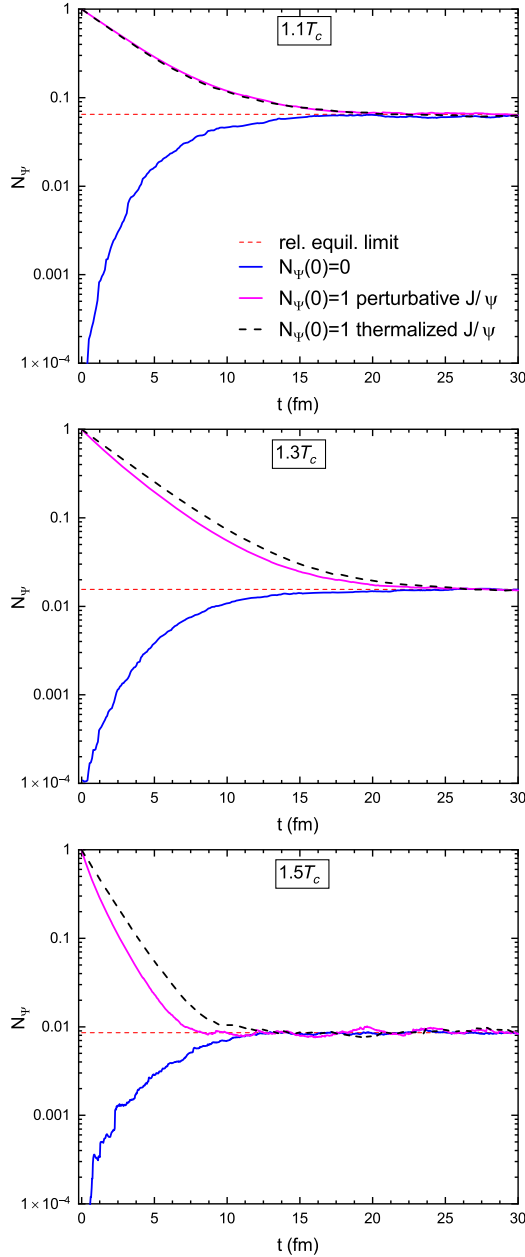


FIG. 7. The evolution of J/ψ yield for total reaction rates and transported c and $\bar{c}$ with $\gamma = 0.4 \text{ fm}^{-1}$ at $1.1T_c$ (top), $1.3T_c$ (middle), and $1.5T_c$ (bottom). Different initial conditions are compared. The horizontal red dashed lines are the same as shown in Figs. 3 and 5.

from perturbative calculations in $\sqrt{s} = 5.02 \text{ TeV}$ proton-proton collisions [28,58]. The results are shown in Fig. 7 for three temperatures. Now, with the total quarkonium reaction rates and larger charm quark thermalization rates, the equilibration time for the J/ψ yield generally comes to the order of 10–15 fm, which is roughly comparable to the lifetime of QGP created in the most central Pb-Pb collisions at the LHC energies. This equilibration time is not very sensitive to the temperatures explored, nor to the choice of

initial conditions. For the latter, when there is one bound state initially [$N_\psi(0) = 1$], we have compared the results from using two kinds of momentum distributions (perturbative [28] vs thermalized) for that bound state at the beginning. It turns out that at $1.3T_c$ and $1.5T_c$, where the NLO dissociation rates (increasing with momentum, cf. Fig. 1) dominate, the perturbative momentum distribution that entails a larger mean momentum permits a faster equilibration (solid purple curve in Fig. 7) than the case with thermal momentum distribution (dashed black curve).

V. SUMMARY

In this work, we have established a semiclassical transport framework to simulate heavy quarkonium chemical equilibration through regeneration and dissociation dynamics in the QGP, including the leading-order $2 \leftrightarrow 2$ and next-to-leading-order $2 \leftrightarrow 3$ processes. The scattering amplitudes are taken from our perturbative calculations [17,48] using color-electric dipole coupling vertex from QCD multipole expansion. Utilizing the test-particle representations for the heavy quark distribution, the Boltzmann equation describing the time evolution of quarkonium distributions was reduced to tractable iteration schemes for the dissociation of a moving quarkonium in QGP and the regeneration from uncorrelated heavy quark and anti-quark pairs.

Numerically, we first simulated the quarkonium (the ground state charmonium J/ψ) equilibration in a static and homogeneous QGP box by assuming fully thermalized distributions for heavy quarks participating in recombination. As expected from the rate equations [Eqs. (16) and (19)], given sufficiently long time, the integrated yields of J/ψ can always reach the equilibrium limit as governed by the statistical balance equation (7), regardless of the initial number of bound states. Different speeds toward the equilibrium limit were also compared for various LO and NLO reactions at different temperatures. Next, we considered a more realistic case, in which heavy quarks and antiquarks are not thermalized from the beginning but undergo diffusion and gradual thermalization as simulated by Langevin equations. The quarkonium Boltzmann transport is then coupled with the heavy quark diffusion in a real-time fashion. The yields of quarkonia were shown to reach the expected equilibrium limits as well and their final momentum spectra also exhibited good agreement with the analytical Boltzmann distributions, for various LO and NLO reactions. Yet the equilibration time generally becomes significantly longer than the former case, because now the regeneration rates involving nonequilibrium heavy quarks in the early stages of the evolution are suppressed compared to the case with completely thermalized heavy quarks, highlighting the interplay between the open and hidden charm sector in quantifying the heavy quarkonium equilibration. We have also found that the equilibration time is almost independent of the initial number of bound

state when the reaction rates are sufficiently large. With total quarkonium reaction rates and more realistic charm quark thermal relaxation rate ($\gamma \sim 0.4 \text{ fm}^{-1}$), the equilibration time reduces to the order of 10–15 fm that is comparable to the QGP lifetime in central heavy-ion collisions at the LHC energies. We note that the reaction rates used in the present work are taken from perturbative calculations [17,48], which may be further enhanced by some nonperturbative mechanism [60–62]. Should larger reaction rates be used, one expects the heavy quarkonium equilibration time to be further reduced, thereby lending a more quantitative understanding of reaction dynamics underlying the statistical hadronization model [7–9] for charmonium production in heavy-ion collisions.

This work paves the way for realistic phenomenological applications to heavy quarkonium transport [63]. For this, the approach developed here in a static and homogeneous QGP box needs to be extended to incorporate a dynamically evolving medium usually simulated by relativistic hydrodynamics, in which the heavy quarkonium dissociation and regeneration dynamics is to be coupled to the single heavy quark diffusion in a real-time fashion. This

would enable us to study the production of heavy quarkonia in heavy-ion collisions in a fully dynamical way, even taking into account the quantum transitions between different bound states [17].

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (NSFC) under Grant No. 12475141, the Postgraduate Research and Practice Innovation Program of Jiangsu Province under No. KYCX25_0676, and the Fundamental Research Funds for the Central Universities No. 30925020109.

DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

-
- [1] J. Zhao, K. Zhou, S. Chen, and P. Zhuang, *Prog. Part. Nucl. Phys.* **114**, 103801 (2020).
 - [2] M. He, H. van Hees, and R. Rapp, *Prog. Part. Nucl. Phys.* **130**, 104020 (2023).
 - [3] A. Andronic, P. B. Gossiaux, P. Petreczky, R. Rapp, M. Strickland, J. P. Blaizot, N. Brambilla, P. Braun-Munzinger, B. Chen, S. Delorme *et al.*, *Eur. Phys. J. A* **60**, 88 (2024).
 - [4] T. Matsui and H. Satz, *Phys. Lett. B* **178**, 416 (1986).
 - [5] L. Kluberg and H. Satz, *arXiv:0901.3831*.
 - [6] A. Tumasyan *et al.* (CMS Collaboration), *Phys. Rev. Lett.* **133**, 022302 (2024).
 - [7] A. Andronic, P. Braun-Munzinger, K. Redlich, and J. Stachel, *Nature (London)* **561**, 321 (2018).
 - [8] A. Andronic, P. Braun-Munzinger, M. K. Köhler, A. Mazeliauskas, K. Redlich, J. Stachel, and V. Vislavicius, *J. High Energy Phys.* **07** (2021) 035.
 - [9] A. Andronic and R. Arnaldi, *arXiv:2501.08290*.
 - [10] M. E. Peskin, *Nucl. Phys.* **B156**, 365 (1979).
 - [11] G. Bhanot and M. E. Peskin, *Nucl. Phys.* **B156**, 391 (1979).
 - [12] L. Grandchamp and R. Rapp, *Phys. Lett. B* **523**, 60 (2001).
 - [13] T. Song and S. H. Lee, *Phys. Rev. D* **72**, 034002 (2005).
 - [14] J. Hong and S. H. Lee, *Phys. Rev. C* **99**, 034905 (2019).
 - [15] S. Chen and M. He, *Phys. Lett. B* **786**, 260 (2018).
 - [16] X. Yao and B. Müller, *Phys. Rev. D* **100**, 014008 (2019).
 - [17] S. Zhao and M. He, *Phys. Rev. D* **110**, 074040 (2024).
 - [18] M. Laine, O. Philipsen, P. Romatschke, and M. Tassler, *J. High Energy Phys.* **03** (2007) 054.
 - [19] A. Beraudo, J. P. Blaizot, and C. Ratti, *Nucl. Phys.* **A806**, 312 (2008).
 - [20] N. Brambilla, M. A. Escobedo, J. Ghiglieri, and A. Vairo, *J. High Energy Phys.* **05** (2013) 130.
 - [21] P. Braun-Munzinger and J. Stachel, *Phys. Lett. B* **490**, 196 (2000).
 - [22] R. L. Thews, M. Schroedter, and J. Rafelski, *Phys. Rev. C* **63**, 054905 (2001).
 - [23] L. Grandchamp, R. Rapp, and G. E. Brown, *Phys. Rev. Lett.* **92**, 212301 (2004).
 - [24] S. Acharya *et al.* (ALICE Collaboration), *Phys. Lett. B* **849**, 138451 (2024).
 - [25] S. Acharya *et al.* (ALICE Collaboration), *J. High Energy Phys.* **10** (2020) 141.
 - [26] A. Tumasyan *et al.* (CMS Collaboration), *Phys. Rev. Lett.* **128**, 252301 (2022).
 - [27] K. Zhou, N. Xu, Z. Xu, and P. Zhuang, *Phys. Rev. C* **89**, 054911 (2014).
 - [28] M. He, B. Wu, and R. Rapp, *Phys. Rev. Lett.* **128**, 162301 (2022).
 - [29] B. Wu, Z. Tang, M. He, and R. Rapp, *Phys. Rev. C* **109**, 014906 (2024).
 - [30] S. Zhao and M. He, *Phys. Lett. B* **861**, 139283 (2025).
 - [31] A. Polleri, T. Renk, R. Schneider, and W. Weise, *Phys. Rev. C* **70**, 044906 (2004).
 - [32] X. Yao and B. Müller, *Phys. Rev. C* **97**, 014908 (2018); **97**, 049903(E) (2018).
 - [33] T. Song, K. C. Han, and C. M. Ko, *Phys. Rev. C* **85**, 054905 (2012).
 - [34] X. Du and R. Rapp, *Phys. Lett. B* **834**, 137414 (2022).
 - [35] J. Hong and S. H. Lee, *Phys. Lett. B* **801**, 135147 (2020).

- [36] X. Yao, W. Ke, Y. Xu, S. A. Bass, and B. Müller, *J. High Energy Phys.* **01** (2021) 046.
- [37] X. Du, M. He, and R. Rapp, *Phys. Rev. C* **96**, 054901 (2017).
- [38] N. Brambilla, M. A. Escobedo, J. Soto, and A. Vairo, *Phys. Rev. D* **96**, 034021 (2017).
- [39] Y. Akamatsu, *Prog. Part. Nucl. Phys.* **123**, 103932 (2022).
- [40] X. Yao, *Int. J. Mod. Phys. A* **36**, 2130010 (2021).
- [41] N. Brambilla, M. A. Escobedo, M. Strickland, A. Vairo, P. Vander Griend, and J. H. Weber, *J. High Energy Phys.* **05** (2021) 136.
- [42] T. Miura, Y. Akamatsu, M. Asakawa, and A. Rothkopf, *Phys. Rev. D* **101**, 034011 (2020).
- [43] T. Miura, Y. Akamatsu, M. Asakawa, and Y. Kaida, *Phys. Rev. D* **106**, 074001 (2022).
- [44] N. Brambilla, T. Magorsch, and A. Vairo, *arXiv:2508.11743*.
- [45] X. Yao and T. Mehen, *Phys. Rev. D* **99**, 096028 (2019).
- [46] C. Young and E. Shuryak, *Phys. Rev. C* **79**, 034907 (2009).
- [47] N. Oei, N. Krenz, H. van Hees, C. Greiner, and J. M. Torres-Rincon, *Phys. Rev. D* **111**, 074012 (2025).
- [48] S. Chen and M. He, *Phys. Rev. C* **96**, 034901 (2017).
- [49] T. M. Yan, *Phys. Rev. D* **22**, 1652 (1980).
- [50] N. Brambilla, A. Pineda, J. Soto, and A. Vairo, *Rev. Mod. Phys.* **77**, 1423 (2005).
- [51] Y. Sumino, *arXiv:1411.7853*.
- [52] S. Weinberg, *The Quantum Theory of Fields. Vol. 1: Foundations* (Cambridge University Press, Cambridge, England, 2005).
- [53] M. D. Schwartz, *Quantum Field Theory and the Standard Model* (Cambridge University Press, Cambridge, England, 2014).
- [54] F. Karsch, M. T. Mehr, and H. Satz, *Z. Phys. C* **37**, 617 (1988).
- [55] R. Rapp, D. Blaschke, and P. Crochet, *Prog. Part. Nucl. Phys.* **65**, 209 (2010).
- [56] N. Brambilla, M. A. Escobedo, J. Ghiglieri, and A. Vairo, *J. High Energy Phys.* **12** (2011) 116.
- [57] M. He, H. van Hees, P. B. Gossiaux, R. J. Fries, and R. Rapp, *Phys. Rev. E* **88**, 032138 (2013).
- [58] M. He and R. Rapp, *Phys. Rev. Lett.* **124**, 042301 (2020).
- [59] Z. Tang and R. Rapp, *Phys. Rev. C* **108**, 044906 (2023).
- [60] B. Scheiing-Hitschfeld and X. Yao, *Phys. Rev. D* **108**, 054024 (2023); **109**, 099902(E) (2024).
- [61] G. Nijs, B. Scheiing-Hitschfeld, and X. Yao, *Phys. Rev. D* **109**, 094043 (2024).
- [62] Z. Tang, S. Mukherjee, P. Petreczky, and R. Rapp, *Phys. Rev. D* **112**, 034030 (2025).
- [63] J. Chen, J. H. Chen, X. Dong, X. He, X. H. He, H. Huang, H. Z. Huang, F. Liu, X. Luo, X. F. Luo *et al.*, *Nucl. Sci. Tech.* **35**, 214 (2024).