Quarkonium in medium
an EFT and open quantum system description

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Based on

(1) N. Brambilla, M.A. Escobedo, M. Strickland, A. Vairo, P. Vander Giemen and J.H. Weber

Bottomonium production in heavy-ion collisions using quantum trajectories: Differential observables and momentum anisotropy
arXiv:2107.06222

(2) N. Brambilla, M.A. Escobedo, M. Strickland, A. Vairo, P. Vander Giemen and J.H. Weber

Bottomonium suppression in an open quantum system using the quantum trajectories method
JHEP 05 (2021) 136 arXiv:2012.01240

(3) N. Brambilla, M.A. Escobedo, J. Soto and A. Vairo

Heavy quarkonium suppression in a fireball
Phys. Rev. D 97 (2018) 074009 arXiv:1711.04515

(4) N. Brambilla, M.A. Escobedo, J. Soto and A. Vairo

Quarkonium suppression in heavy-ion collisions: an open quantum system approach
Phys. Rev. D 96 (2017) 034021 arXiv:1612.07248
Energy scales

Quarkonium being a composite system is characterized by several energy scales:

- the scales of a non-relativistic bound state
  \( v \) is the relative heavy-quark velocity; \( v \sim \alpha_s \) for a Coulombic bound state:
  - \( M \) (mass),
  - \( M_v \) (momentum transfer, inverse distance),
  - \( M_v^2 \) (kinetic energy, binding energy, potential \( V \)), ...

- the thermodynamical scales:
  - \( T \) (temperature), ...

\( T \) stands for a generic inverse correlation length characterizing the medium.
For definiteness we will assume that the system is locally in thermal equilibrium so that a slowly varying time-dependent temperature can be defined.

The non-relativistic scales are hierarchically ordered: \( M \gg M_v \gg M_v^2 \)
The existence of a hierarchy of energy scales calls for a description of the system in terms of a hierarchy of EFTs. We assume \( T \approx 400 \text{ MeV} < M_v \approx 1.5 \text{ GeV} \) for \( T \).

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Brambilla Pineda Soto Vairo RMP 77 (2005) 1423
Brambilla Ghiglieri Petreczky Vairo PRD 78 (2008) 014017
\[ \mathcal{L} = -\frac{1}{4} F_{\mu
u}^a F^{\mu\nu a} + \sum_{i=1}^{n_f} q_i \bar{\gamma} \tau_i + \int d^4 r \text{Tr} \left\{ S^\dagger (i\partial_0 - h_s) S + O^\dagger (iD_0 - h_o) O \right\} \]

- **LO in** \( r \)

\[ \theta(T) e^{-iT h_s} \quad \theta(T) e^{-iT h_o} \left( e^{-i \int dt A^{a 4)} \right) \]

+ \( V_A \text{Tr} \left\{ O^\dagger r \cdot g E S + S^\dagger r \cdot g E O \right\} + \frac{V_B}{2} \text{Tr} \left\{ O^\dagger r \cdot g E O + O^\dagger r \cdot g E \right\} \)

- **NLO in** \( r \)

\[ O^\dagger r \cdot g E S \quad O^\dagger \{ r \cdot g E, O \} \]

+ \( \cdots \)
pNRQCD: fields and potentials

Fields:
- $S^\dagger$ creates a quark-antiquark pair in a color singlet configuration.
- $O^\dagger$ creates a (unbound) quark-antiquark pair in a color octet configuration.

Potentials:
- quark-antiquark color singlet Hamiltonian $= h_s = \frac{p^2}{M} - \frac{4}{3} \frac{\alpha_s}{r} + \ldots$
- quark-antiquark color octet Hamiltonian $= h_o = \frac{p^2}{M} + \frac{\alpha_s}{6r} + \ldots$
- $V_A = V_B = 1$ up to higher corrections in $\alpha_s$. 
Open quantum system

- **System**: heavy quarks/quarkonium
- **Environment**: quark gluon plasma

We may define a (reduced) density matrix in pNRQCD for the heavy quark-antiquark pair in a color singlet and octet configuration:

\[
\langle r', R' | \rho_s(t'; t) | r, R \rangle \equiv \text{Tr} \left\{ \rho_{\text{full}}(t_0) S^\dagger(t, r, R) S(t', r', R') \right\}
\]

\[
\langle r', R' | \rho_o(t'; t) | r, R \rangle \frac{\delta_{ab}}{8} \equiv \text{Tr} \left\{ \rho_{\text{full}}(t_0) O^a(t, r, R) O^b(t', r', R') \right\}
\]

\[t_0 \approx 0.6 \text{ fm} \] is the time formation of the plasma.

The system is in non-equilibrium because through interaction with the environment (quark gluon plasma) singlet and octet quark-antiquark states continuously transform in each other although the number of heavy quarks is conserved: \( \text{Tr}\{\rho_s\} + \text{Tr}\{\rho_o\} = 1. \)
Closed-time path formalism

In the closed-time path formalism we can represent the density matrices as 12 propagators on a closed time path:

\[
\langle r', R' | \rho_s(t'; t) | r, R \rangle = \langle S_1(t', r', R') S_2^\dagger(t, r, R) \rangle
\]

\[
\langle r', R' | \rho_0(t'; t) | r, R \rangle \frac{\delta_{ab}}{8} = \langle O_b^1(t', r', R') O_a^2(t, r, R) \rangle
\]

\[
\langle r', R' | \rho_s(t'; t) | r, R \rangle = \langle S_1(t', r', R') S_2^\dagger(t, r, R) \rangle
\]

\[
\langle r', R' | \rho_0(t'; t) | r, R \rangle \frac{\delta_{ab}}{8} = \langle O_b^1(t', r', R') O_a^2(t, r, R) \rangle
\]

Differently from the thermal equilibrium case 12 propagators are relevant (in thermal equilibrium they are exponentially suppressed).

12 propagators are not time ordered, while 11 and 22 operators select the forward time direction \( \propto \theta(t - t') \), \( \theta(t' - t) \).
Expansions

- The density of heavy quarks is much smaller than the one of the light d.o.f.: we expand at first order in the heavy quark-antiquark density.

- We consider $T$ much smaller than the inverse Bohr radius of the quarkonium: we expand up to order $r^2$ in the multipole expansion.

The evolution depends on the density at initial time: non Markovian evolution.
Resummation

Resumming \((t - t_0) \times \text{self-energy contributions} \ldots\)

(Resummation is accurate at order \(r^2\) and consistent with unitary evolution in the absence of dissipation.)
... and differentiating over time we obtain the coupled evolution equations:

\[
\frac{d\rho_s(t; t)}{dt} = -i [h_s, \rho_s(t; t)] - \Sigma_s(t) \rho_s(t; t) - \rho_s(t; t) \Sigma_s^\dagger(t) + \Xi_{so}(\rho_s(t; t), t)
\]

\[
\frac{d\rho_o(t; t)}{dt} = -i [h_o, \rho_o(t; t)] - \Sigma_o(t) \rho_o(t; t) - \rho_o(t; t) \Sigma_o^\dagger(t) + \Xi_{ao}(\rho_o(t; t), t)
\]

+ \Xi_{oo}(\rho_o(t; t), t)

• The evolution equations are now valid for large time.
• The evolution equations are Markovian.
Interpretation

- The self energies $\Sigma_s$ and $\Sigma_o$ provide the in-medium induced mass shifts, $\delta m_{s,o}$, and widths, $\Gamma_{s,o}$, for the color-singlet and color-octet heavy quark-antiquark pairs respectively:

  \[
  -i \Sigma_{s,o}(t) + i \Sigma_{s,o}^\dagger(t) = 2 \text{Re} (-i \Sigma_{s,o}(t)) = 2 \delta m_{s,o}(t) \\
  \Sigma_{s,o}(t) + \Sigma_{s,o}^\dagger(t) = -2 \text{Im} (-i \Sigma_{s,o}(t)) = \Gamma_{s,o}(t)
  \]

- $\Xi_{so}$ accounts for the production of singlets through the decay of octets, and $\Xi_{os}$ and $\Xi_{oo}$ account for the production of octets through the decays of singlets and octets respectively. There are two octet production mechanisms/octet chromoelectric dipole vertices in the pNRQCD Lagrangian.

- The conservation of the trace of the sum of the densities, i.e., the conservation of the number of heavy quarks, follows from

  \[
  \text{Tr} \left\{ \rho_s(t; t) \left( \Sigma_s(t) + \Sigma_s^\dagger(t) \right) \right\} = \text{Tr} \left\{ \Xi_{os} (\rho_s(t; t), t) \right\} \\
  \text{Tr} \left\{ \rho_o(t; t) \left( \Sigma_o(t) + \Sigma_o^\dagger(t) \right) \right\} = \text{Tr} \left\{ \Xi_{so} (\rho_o(t; t), t) + \Xi_{oo} (\rho_o(t; t), t) \right\}
  \]
An alternative way of writing the evolution equations is

\[
\frac{d\rho}{dt} = -i[H, \rho] + \sum_{nm} h_{nm} \left( L_i^n \rho L_i^m \dagger - \frac{1}{2} \{ L_i^m \dagger L_i^n, \rho \} \right)
\]

\[
\rho = \begin{pmatrix} \rho_s & 0 \\ 0 & \rho_o \end{pmatrix} \quad H = \begin{pmatrix} h_s + \frac{\Sigma_s - \Sigma_s^\dagger}{2i} & 0 \\ 0 & h_o + \frac{\Sigma_o - \Sigma_o^\dagger}{2i} \end{pmatrix}
\]

\[
\Sigma_s(t) = r^i A_i^{so \dagger}(t) \quad \Sigma_o(t) = \frac{r^i A_i^{so \dagger}(t)}{8} + \frac{5}{16} A_i^{so \dagger}(t)
\]

\[
L_i^0 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} r^i \quad L_i^1 = \begin{pmatrix} 0 & 0 \\ 0 & \frac{5}{16} A_i^{so \dagger} \end{pmatrix}
\]

\[
L_i^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} r^i \quad L_i^3 = \begin{pmatrix} 0 & 1/8 A_i^{so \dagger} \\ A_i^{so \dagger} & 0 \end{pmatrix}
\]

with \( A_i^{so}(t) = \frac{g^2}{6} \int_{t_0}^{t} dt_2 e^{ih_s(t_2-e-t)} r^i e^{ih_o(t-t_2)} \langle E_{a,j}(t_2,0) E_{a,i}(t,0) \rangle \).
Positivity

The matrix $h_{nm}$ is

$$h = \begin{pmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{pmatrix}$$

If $h$ were a positive definite matrix then it would always be possible to redefine the operators $L_1^n$ in such a way that the evolution equation would be of the Lindblad form.

Since, however, $h$ is not a positive definite matrix, the Lindblad theorem does not guarantee that the equations may be brought into a Lindblad form.

A special case is the strongly-coupled case. There $L_1^n \propto L_3^n$ and $L_2^n \propto L_3^n$, which allows to set to zero, after a redefinition of $L_1^n$, the eigenvectors of $h$ associated with negative eigenvalues, eventually leading to an evolution equation of the Lindblad form.
Time scales

Environment correlation time: \( \tau_E \sim \frac{1}{T} \)

System intrinsic time scale: \( \tau_S \sim \frac{1}{E} \)

System relaxation time: \( \tau_R \sim \frac{1}{\text{self-energy}} \sim \frac{1}{a_0 a_0^2 \Lambda^3} \quad a_0 = \text{Bohr radius, } \Lambda = T, E \)

- Because we have assumed \( 1/a_0 \gg \Lambda \), it follows \( \tau_R \gg \tau_S, \tau_E \)
  which, after resummation \( (t - t_0 \gg \tau_R) \), qualifies the system as Markovian.

- If \( T \gg E \) then \( \tau_S \gg \tau_E \)
  which qualifies the motion of the system as quantum Brownian.

\[ \text{Akamatsu PRD 91 (2015) 056002} \]
From the evolution equations to the Lindblad equation

Under the Markovian
$$\tau_R \gg \tau_S, \tau_E \quad \text{or} \quad \frac{1}{a_0} \gg E, T$$

and quantum Brownian motion condition
$$\tau_S \gg \tau_E \quad \text{or} \quad T \gg E$$

at (N)LO in $E/T$ the evolution equations can be written in the Lindblad form.
Heavy quark-antiquarks in a strongly coupled medium

If $E \ll T$ the Lindblad equation for a strongly coupled plasma reads

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_i (C_i \rho C_i^\dagger - \frac{1}{2} \{C_i^\dagger C_i, \rho\})$$

$$\rho = \begin{pmatrix} \rho_s & 0 \\ 0 & \rho_o \end{pmatrix}$$

$$H = \begin{pmatrix} h_s & 0 \\ 0 & h_o \end{pmatrix} + \frac{r^2}{2} \gamma(t) \begin{pmatrix} 1 & 0 \\ 0 & \frac{7}{16} \end{pmatrix}$$

$$C_i^0 = \sqrt{\frac{r(t)}{8}} r_i \begin{pmatrix} 0 & 1 \\ \frac{1}{\sqrt{8}} & 0 \end{pmatrix}, \quad C_i^1 = \sqrt{\frac{5r(t)}{16}} r_i \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$
Thermal width and mass shift

The quantity $\kappa$ is related to the thermal decay width of the heavy quarkonium. In particular for $1S$ states, we have

$$\Gamma(1S) = -2\langle \text{Im} \ (-i\Sigma_s) \rangle = 3a_0^2 \kappa$$

The quantity $\gamma$ is related to the thermal mass shift of the heavy quarkonium. In particular for $1S$ states, we have

$$\delta M(1S) = \langle \text{Re} \ (-i\Sigma_s) \rangle = \frac{3}{2} a_0^2 \gamma$$
Low energy parameters may be determined by numerical calculations in lattice QCD. \( \kappa \) is the heavy-quark momentum diffusion coefficient:

\[
\kappa = \frac{g^2}{18} \operatorname{Re} \int_{-\infty}^{+\infty} ds \left< T E^{a,i}(s,0) \phi^{ab}(s,0) E^{b,j}(0,0) \right> 
\]
\[ \gamma = \frac{g^2}{18} \ln \left( \int_{-\infty}^{+\infty} ds \braket{T E^{a, i}(s, 0) \phi^{a b}(s, 0) E^{b, i}(0, 0)} \right) \]

- $J/\psi, T = 251$ MeV
- $\Upsilon(1S), T = 407$ MeV
- $\Upsilon(1S), T = 251$ MeV
- $n_f = 3, T = 407$ MeV (perturbation theory)
- $n_f = 3, T = 251$ MeV (perturbation theory)

*R Brambilla Escobedo Vairo Vander Griend* PRD 100 (2019) 054025

*from the lattice data of Kim Petreczky Rothkopf* JHEP 11 (2018) 088

*for an Euclidean version Eller Ghiglieri Moore* PRD 99 (2019) 094042
Evolution set up

- After heavy-ion collision, heavy quark-antiquarks propagate freely up to 0.6 fm.
- From 0.6 fm to the freeze-out time $t_F$ they propagate in medium.
- We assume the medium to be locally in thermal equilibrium.
- We use a 3+1D dissipative relativistic hydrodynamics code that makes use of the quasiparticle anisotropic hydrodynamics (aHydroQP) framework. The code uses a realistic equation of state fit to lattice QCD measurements and is tuned to soft hadronic data collected in 5.02 TeV collisions using smooth optical Glauber initial conditions.
  - Alqahtani Nopoush Strickland PRC 92 (2015) 054910, 95 (2017) 034906
  - Alqahtani Nopoush Strickland PPNP 101 (2018) 204
Quantum trajectories algorithm

The QTraj code implements the quantum trajectories algorithm and the waiting time approach as follows.

1. Initialize a wave function $|\psi(t_0)\rangle$ at initial time $t_0$, which corresponds to the initial quantum state of the particle given by $\rho(t_0) = |\psi(t_0)\rangle\langle\psi(t_0)|$.

2. Generate a random number $0 < r_1 < 1$ and evolve the wave function forward in time with $H_{\text{eff}}$ until $|e^{-\frac{i}{\hbar}\int_{t_0}^{t} H_{\text{eff}}(t') dt'} |\psi(t_0)\rangle |^2 \leq r_1$ where $H_{\text{eff}} = H - i\Gamma/2$, $\Gamma = \sum \Gamma_n$ and $\Gamma_n = C_n^\dagger C_n$. Denote the first time step fulfilling the inequality as the jump time $t_j$. If the jump time is greater than the simulation run time $t_F$, end the simulation at time $t_F$; otherwise, proceed to step 3.

3. At time $t_j$, initiate a quantum jump:
   
   (a) If the system is in a singlet configuration, jump to octet. If the system is in an octet configuration, generate a random number $0 < r_2 < 1$ and jump to singlet if $r_2 < 2/7$; otherwise, remain in the octet configuration.

   (b) Generate a random number $0 < r_3 < 1$; if $r_3 < l/(2l + 1)$, take $l \rightarrow l - 1$; otherwise, take $l \rightarrow l + 1$.

   (c) Multiply the wavefunction by $r$ and normalize.

4. Continue from step 2.

Ba Omar Escobedo Islam Strickland Thapa Vander Griend Weber arXiv:2107.06147
Jumps and probabilities

The probabilities in step 3 correspond to the branching fractions into a state of different color and/or angular momentum:

\[ p_n = \frac{\langle \psi(t)|\Gamma_n|\psi(t)\rangle}{\langle \psi(t)|\Gamma|\psi(t)\rangle} \]

Each evolution of the wave function from time \( t_0 \) to \( t_F \) is called a quantum trajectory. In practice, a large number of quantum trajectories must be generated. As the number of trajectories considered increases, the average converges to the solution of the Lindblad equation.

- Dalibard Castin Molmer PRL 68 (1992) 580
- Daley AP 63 (2014) 77
Simulation set up

We employ a radial lattice of NUM = 4096 lattice sites and a radial length of L = 80 GeV$^{-1}$, corresponding to a radial lattice spacing of $a \approx 0.0195$ GeV$^{-1}$. The real time integration is discretized with a time step of $dt = 0.001$ GeV$^{-1}$.

We sample approximately $7 \times 9 \times 10^5$ independent physical trajectories for each choice of $\kappa(T)/T^3$ and $\gamma/T^3$, with approximately 50-100 quantum trajectories per physical trajectory. To generate each physical trajectory, we sample the bottomonium production point in the transverse plane using the nuclear binary collision overlap profile $N_{AA}^{\text{bin}}(x, y, b)$, the initial transverse momentum of the state $p_T$ from an $E_T^{-4}$ spectrum, and the initial azimuthal angle $\phi$ of the state’s momentum uniformly in $[0, 2\pi)$. We bin the results for the survival probability as a function of centrality, $p_T$, and $\phi$. This allows us to make predictions for differential observables such as $R_{AA}$ as a function of $p_T$ and elliptic flow.

To ensure that the hierarchy of energy scales of the EFT is fulfilled, we evolve the state in the vacuum when the temperature falls below $T_F = 250$ MeV.
We compute the nuclear modification factor \( R_{AA} \) from

\[
R_{AA}(nS) = \frac{\langle n, q | \rho_s(t_F, t_F') | n, q \rangle}{\langle n, q | \rho_s(0, 0) | n, q \rangle}
\]
Bottomonium nuclear modification factor vs $p_T$
Double ratio $R_{AA}[\Upsilon(2S)]$ to $R_{AA}[\Upsilon(1S)]$
Double ratio $R_{AA}[\Upsilon(2S)]$ to $R_{AA}[\Upsilon(1S)]$ vs $p_T$
Double ratio $R_{AA}[\Upsilon(3S)]$ to $R_{AA}[\Upsilon(1S)]$
Elliptic flow $v_2$ of the $\Upsilon(1S)$
Elliptic flow $v_2$ of the $\Upsilon(1S)$ vs $p_T$
Elliptic flow $v_2$ of the $\Upsilon(2S)$ and $\Upsilon(3S)$
Conclusions

We have shown how the heavy quark-antiquark pair out-of-equilibrium evolution can be treated in the framework of pNRQCD. With respect to previous determinations:

- the medium may be a strongly-coupled plasma (not necessarily a quark-gluon plasma) whose characteristics are determined by lattice calculations;
- the total number of heavy quarks, i.e., $\text{Tr}\{\rho_s\} + \text{Tr}\{\rho_o\}$, is preserved by the evolution equations;
- the non-abelian nature of QCD is fully accounted for;
- the treatment does not rely on classical approximations.

The evolution equations follow from assuming the inverse size of the quark-antiquark system to be larger than any other scale of the medium and from being accurate at first non-trivial order in the multipole expansion and at first order in the heavy-quark density.

Under some conditions (large time, quasistatic evolution, quantum Brownian motion) the evolution equations are of the Lindblad form. Their numerical solution provides $R_{AA}[T(nS)]$ and differential observables in good agreement with LHC data.