Nonequilibrium evolution of bottomonium in QGP
Quark-Gluon Plasma Characterization with Heavy Flavor Probes

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Introduction

Motivation: use heavy quarks and their bound states to probe the strongly coupled medium formed in heavy ion collisions

- high mass $M$ of bottom quarks and the short formation time of their bound states make them ideal probes of the quark gluon plasma (QGP); observables of interest include nuclear suppression factor $R_{AA}$ and elliptic flow $v_2$

- ideally suited for treatment using the formalism of open quantum systems (OQS) and effective field theory (EFT)
  - OQS: allows for the rigorous treatment of a quantum system of interest (heavy quarkonium) coupled to an environment (QGP)
  - EFTs: take advantage of the large mass of the heavy quark and the resulting nonrelativistic nature of the system and small bound state radius using potential nonrelativistic QCD (pNRQCD), an EFT of the strong interaction

Advantages: fully quantum, non-Abelian, heavy quark number conserving, account for dissociation and recombination, and valid for strong or weak coupling
Physical Setup

relevant energy scales (EFT)

▶ heavy quark mass $M = M_b \sim 5$ GeV
▶ inverse Bohr radius $1/a_0 \sim 1.5$ GeV
▶ $(\pi$ times) the temperature of the medium $(\pi)T \sim 1.5$ GeV
▶ (Coulombic) binding energy $E \sim 0.5$ GeV
▶ hierarchical ordering: $M \gg 1/a_0 \gg (\pi)T \gg E$ \(^{1}\)

relevant time scales (OQS)

▶ system intrinsic time scale: $\tau_S \sim 1/E$
▶ environment correlation time: $\tau_E \sim 1/(\pi T)$
▶ relaxation time: $\tau_R \sim 1/\Sigma_s \sim 1/(a_0^2(\pi T)^3)$ (where $\Sigma_s$ is the thermal self energy)

\(^{1}\pi T \sim 1.5$ GeV at initial time; medium quickly expands and cools such that $1/a_0 \gg \pi T$ is realized
Hierarchies and Simplifying Assumptions

quantum Brownian motion for

$$\tau_R, \tau_S \gg \tau_E,$$

where $\tau_R$, $\tau_S$, and $\tau_E$ are the relaxation, system intrinsic, and environment correlation time scales, respectively, the system realizes quantum Brownian motion

Simplifying Approximations

hierarchy of scales allows for two simplifying approximations:

- **Born approximation**: quarkonium has little effect on the medium at time scales of interest; density matrix factorizes, i.e., $\rho(t) \propto \rho_S(t) \otimes \rho_E$

- **Markov approximation**: only the state of the quarkonium at the present time is necessary to describe its evolution, i.e., no memory integral
potential Non-Relativistic QCD (pNRQCD)

- effective theory of the strong interaction obtained from full QCD via non-relativistic QCD (NRQCD) by successive integrating out of the hard ($M$) and soft ($Mv$) scales where $v \ll 1$ is the relative velocity in a heavy-heavy bound state

- degrees of freedom are singlet and octet heavy-heavy bound states and ultrasoft gluons

- small bound state radius and large quark mass allow for double expansion in $r$ and $M^{-1}$ at the Lagrangian level
\[ \mathcal{L}_{pNRQCD} = \text{Tr} \left[ S^\dagger (i\partial_0 - h_s) S + O^\dagger (iD_0 - h_o) O + O^\dagger r \cdot g E S \\
+ S^\dagger r \cdot g E O + \frac{1}{2} O^\dagger \{ r \cdot g E, O \} \right] \]

- singlet and octet field \( S \) and \( O \) interacting via chromo-electric dipole vertices
- \( h_{s,o} = \frac{p^2}{M} + V_{s,o} \): singlet, octet Hamiltonian
  - \( V_s = -\frac{C_f \alpha_s (1/a_0)}{r} \): attractive singlet potential
  - \( V_o = \frac{\alpha_s (1/a_0)}{2N_c r} \): repulsive octet potential
- \( iD_0 O = i\partial_0 O - [gA_0, O] \)
  - commutator can be eliminated via field redefinition

\[ E^{a,i}(s, 0) \rightarrow \tilde{E}^{a,i}(s, 0) = \Omega(s) E^{a,i}(s, 0) \Omega(s)^\dagger \]

where

\[ \Omega(s) = \exp \left[ -ig \int_{-\infty}^{s} ds' A_0(s', 0) \right] \]
evolution equations of in-medium Coulombic heavy quarkonium given by:

\[
\frac{d\rho_s(t)}{dt} = -i [h_s, \rho_s(t)] - \Sigma_s \rho_s(t) - \rho_s(t)\Sigma^\dagger_s + \Xi_{so}(\rho_o(t)) \\
\frac{d\rho_o(t)}{dt} = -i [h_o, \rho_o(t)] - \Sigma_o \rho_o(t) - \rho_o(t)\Sigma^\dagger_o + \Xi_{os}(\rho_s(t)) \\
+ \Xi_{oo}(\rho_o(t))
\]

where the $\Sigma$ and $\Xi$ encode interactions with the medium and can be computed diagrammatically in pNRQCD

\[\text{Evolution Equations}^2\]
Diagrammatic Evolution of $\rho_s(t)$

singlet evolution given by

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

where

$\Sigma_s \rho_s(t) \sim$

$\Xi_{so}(\rho_o(t)) \sim$
Diagramatic Evolution of $\rho_o(t)$

octet evolution given by

$$\frac{d\rho_o(t)}{dt} = -i [h_o, \rho_o(t)] - \Sigma_o \rho_o(t) - \rho_o(t) \Sigma_o^\dagger + \Xi_{os}(\rho_s(t)) + \Xi_{oo}(\rho_o(t))$$

where

$\Sigma_o \rho_o(t) \sim$

$\Xi_{os}(\rho_s(t)) \sim$

$\Xi_{oo}(\rho_o(t)) \sim$
Master Equation

Evolution equations can be rewritten as master equation

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

where

$$\rho(t) = \begin{pmatrix} \rho_s(t) & 0 \\ 0 & \rho_o(t) \end{pmatrix}, \quad H = \begin{pmatrix} h_s + \text{Im}(\Sigma_s) & 0 \\ 0 & h_o + \text{Im}(\Sigma_o) \end{pmatrix},$$

$$L^0_i = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} r_i, \quad L^1_i = \begin{pmatrix} 0 & 0 \\ 0 & \frac{N_c^2 - 4}{2(N_c^2 - 1)} A_i^{oo\dagger} \end{pmatrix}, \quad L^2_i = \begin{pmatrix} 0 & \frac{1}{\sqrt{N_c^2 - 1}} \\ 1 & 0 \end{pmatrix} r_i,$$

$$L^3_i = \begin{pmatrix} 0 & \frac{1}{\sqrt{N_c^2 - 1}} A_i^{os\dagger} \\ A_i^{so\dagger} & 0 \end{pmatrix}, \quad h = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$A_i^{uv} = \frac{g^2}{6N_c} \int_0^\infty ds e^{-i h_u s} r_i e^{i h_v s} \left\langle \tilde{E}^{a,j}(0, 0) \tilde{E}^{a,j}(s, 0) \right\rangle$$
Lindblad Equation

▶ for \((\pi) T \gtrsim E\), \(e^{-ihs,os} \approx 1 - ih_{s,os}\) and medium interactions simplify

\[
A_{ij}^{uv} = \frac{r_i}{2} (\kappa - i\gamma) + \kappa \left( -\frac{ip_i}{2MT} + \frac{\Delta V_{uv}}{4T} r_i \right),
\]

where

\[
\kappa = \frac{g^2}{6N_c} \int_0^\infty dt \langle \{ \tilde{E}_i^a(t, 0), \tilde{E}_i^a(0, 0) \} \rangle,
\]

\[
\gamma = -\frac{ig^2}{6N_c} \int_0^\infty dt \langle \left[ \tilde{E}_i^a(t, 0), \tilde{E}_i^a(0, 0) \right] \rangle,
\]

\[
\frac{\kappa}{4T} = \frac{ig^2}{6N_c} \int_0^\infty dt t \langle \tilde{E}_i^a(t, 0)\tilde{E}_i^a(0, 0) \rangle
\]

▶ \(\kappa\) is the momentum diffusion coefficient occurring in a Langevin equation describing the diffusion of a heavy particle\(^3\); \(\gamma\) is its dispersive counterpart

\(^3\)Phys. Rev. D 74 (2006) 085012 (Casalderrey-Solana, Teaney)
Lindblad Equation at order \((E/T)^0\)

at order 0 in the \(E/T\) expansion, evolution equations can be brought into form of a Lindblad equation

\[
\frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \sum_n \left( C_i^n \rho(t) C_i^{n\dagger} - \frac{1}{2} \{ C_i^{n\dagger} C_i^n, \rho(t) \} \right)
\]

where \(H\) is the quarkonium Hamiltonian, and the \(C^n\) are collapse operators resulting from interactions with the medium

\[
\rho = \begin{pmatrix} \rho_s & 0 \\ 0 & \rho_o \end{pmatrix}, \quad H = \begin{pmatrix} h_s & 0 \\ 0 & h_o \end{pmatrix} + \frac{r^2}{2\gamma} \begin{pmatrix} 1 & 0 \\ 0 & \frac{N_c^2-2}{2(N_c^2-1)} \end{pmatrix},
\]

\[
C_i^0 = \sqrt{\frac{\kappa}{N_c^2-1}} r_i \begin{pmatrix} 0 & 1 \\ \sqrt{N_c^2-1} & 0 \end{pmatrix}, \quad C_i^1 = \sqrt{\frac{(N_c^2-4)\kappa}{2(N_c^2-1)}} r_i \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
\]

medium interactions specified by \(\kappa\) and \(\gamma\)
Lindblad Equation at order \((E/T)^2\)

At order \(E/T\), master equation cannot be written as Lindblad equation; however, we can write a Lindblad equation containing terms up to and including order \((E/T)^2\) equivalent to order \((E/T)\) master equation

\[
H = \begin{pmatrix} h_s & 0 \\ 0 & h_o \end{pmatrix} + \left( \frac{r^2}{2} \gamma + \frac{\kappa}{4MT} \{r_i, p_i\} \right) \begin{pmatrix} 1 & 0 \\ 0 & \frac{N_c^2-2}{2(N_c^2-1)} \end{pmatrix},
\]

\[
C_i^0 = \sqrt{\frac{\kappa}{N_c^2-1}} \left( r^i + \frac{ip_i}{2MT} + \frac{\Delta V_{os}}{4T} r_i \right) \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \sqrt{\kappa} \left( r^i + \frac{ip_i}{2MT} + \frac{\Delta V_{os}}{4T} r_i \right) \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},
\]

\[
C_i^1 = \sqrt{\frac{(N_c^2-4)\kappa}{2(N_c^2-1)}} \left( r^i + \frac{ip_i}{2MT} \right) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}
\]

Medium interactions still specified by \(\kappa\) and \(\gamma\)
Transport Coefficients

- \( \kappa \) is the heavy quarkonium momentum diffusion coefficient; \( \gamma \) is its dispersive counterpart.
- \( \kappa \) and \( \gamma \) related to in-medium width and mass shift of \( \Upsilon(1S) \):

\[
\Gamma(1S) = 3a_0^2 \kappa, \quad \delta M(1S) = \frac{3}{2}a_0^2 \gamma,
\]

and accessible from unquenched lattice measurements of \( \Gamma \) and \( \delta M \).
- Temperature dependent heavy quark momentum diffusion coefficient \( \kappa(T) \) can be extracted from chromo-electric correlation functions measurable on the lattice which suffer from severe UV noise.
  - Currently, multilevel algorithm allows for noise reduction with pure gauge backgrounds, i.e., quenched measurements.
  - In the future, gradient flow will allow for noise reduction with full QCD, i.e., unquenched measurements.
Extraction of $\kappa$

**Figure:** Direct, quenched lattice measurement of heavy quark momentum diffusion coefficient $\hat{\kappa} = \kappa / T^3$ (Brambilla, Leino, Petreczky, Vairo: Phys. Rev. D 102, 074503 (2020)).

We solve the Lindblad equation using the upper, central, and lower $\hat{\kappa}(T) = \kappa(T) / T^3$ curves.
Extraction of $\gamma$

Figure: Indirect extractions of $\hat{\gamma} = \gamma / T^3$ from unquenched lattice measurements of $\delta M(1S)$ (lattice extractions of $\delta M(1S)$ from JHEP 11 (2018) 088 (Kim, Petreczky, Rothkopf) and Phys.Rev.D 100 (2019) 7, 074506 (Larsen, Meinel, Mukherjee, Petreczky)).

We solve the Lindlbad equation in the range $-3.5 \leq \gamma / T^3 \leq 0$. 

$J/\psi, T = 251$ MeV

$\Upsilon(1S), T = 407$ MeV

$\Upsilon(1S), T = 334$ MeV

$\Upsilon(1S), T = 251$ MeV

$n_f = 3, T = 407$ MeV

(perturbation theory)

$n_f = 3, T = 251$ MeV

( perturbation theory)
Quantum Trajectories Algorithm

- Monte Carlo method to solve the Lindblad equation
- less memory intensive due to use of wave function $|\psi\rangle$ rather than density matrix $\rho$
- absorb quantum number conserving diagonal evolution terms of Lindblad equation into a non-Hermitian effective Hamiltonian

$$H_{\text{eff}} = H - \frac{i}{2} \sum_n C_n^\dagger C_n$$

Lindblad equation becomes

$$\frac{d\rho(t)}{dt} = -i \left( H_{\text{eff}} \rho(t) - \rho(t) H_{\text{eff}}^\dagger \right) + \sum_n C_i^\dagger \rho(t) C_i$$

- $H_{\text{eff}}$ term reduces trace of $\rho$ and preserves quantum numbers of state
- $C_n$ term changes quantum numbers of state and ensure overall evolution is trace preserving
\[ H_{\text{eff}} \text{ Evolution} \]

- evolve wavefunction with \( H_{\text{eff}} \)

\[ |\psi(t + \delta t)\rangle = (1 - iH_{\text{eff}}\delta t)|\psi(t)\rangle \]

- \( H_{\text{eff}} \) evolution preserves quantum numbers of the state and decreases its norm

\[ \langle \psi(t + \delta t)|\psi(t + \delta t)\rangle \approx 1 - i\langle \psi(t)|(H_{\text{eff}} - H_{\text{eff}}^\dagger)|\psi(t)\rangle\delta t = 1 - \delta p \]

where

\[ \delta p = \sum_n \langle \psi(t)|C_n^\dagger C_n|\psi(t)\rangle\delta t = \sum_n \delta p_n \]

- decrease in norm related to probability a change of quantum numbers, implemented by \( C_n|\psi(t)\rangle \), occurs
Monte Carlo

(normalized) evolution of state

\[
|\tilde{\psi}(t + \delta t)\rangle = \begin{cases} 
|\psi(t+\delta t)\rangle \sqrt{1-\delta p} & \text{with probability } 1 - \delta p \\
\frac{C_n|\psi(t)\rangle}{\sqrt{\delta p_n / \delta t}} & \text{with probability } \delta p 
\end{cases}
\]

i.e., with probability \(1 - \delta p\), the state evolves as governed by \(H_{\text{eff}}\), and with probability \(\delta p\), is acted on by the collapse operator \(C_n\) simulation

- generate a random number \(0 < r_1 < 1\)
- evolve state with \(H_{\text{eff}}\) until norm squared \(< r_1\)
- generate additional random number(s) to determine which collapse operator \(C_n\) to apply
Equivalence of Evolution and Convergence

\[ \rho(t + \delta t) = (1 - \delta p) \frac{\left| \psi(t + \delta t) \right> \left< \psi(t + \delta t) \right|}{\sqrt{1 - \delta p}} \frac{\left| \psi(t) \right> \left< \psi(t) \right|}{\sqrt{1 - \delta p}} \]

\[ + \delta p \sum_n \frac{\delta p_n C_n}{\delta p} \frac{\left| \psi(t) \right> \left< \psi(t) \right|}{\sqrt{\delta p_n / \delta t}} \frac{C_n^\dagger}{\sqrt{\delta p_n / \delta t}} \]

\[ = \rho(t) - i [H_{\text{eff}} \rho(t) - \rho(t) H_{\text{eff}}^\dagger] \delta t + \sum_n C_n \rho(t) C_n^\dagger \delta t, \]

as given by Lindblad equation

convergence

- calculate expectation values using evolved state
- evolve many states and average to converge to result of directly solving the Lindblad equation
QTraj Implementation$^4$

1. initialize wave function $|\psi(t_0)\rangle$
2. generate random number $0 < r_1 < 1$, evolve with $H_{\text{eff}}$ until
   \[ \frac{|| e^{-i \int_{t_0}^{t} dt' H_{\text{eff}}(t')} |\psi(t_0)\rangle ||^2}{r_1}, \]
   and initiate a quantum jump
3. quantum jump
   3.1 if singlet, jump to octet; if octet, generate random number $0 < r_2 < 1$ and jump to singlet if $r_2$ less than the branching fraction to singlet; otherwise, remain in octet
   3.2 generate random number $0 < r_3 < 1$; if $r_3 < l/(2l + 1)$, \( l \rightarrow l - 1 \); otherwise, \( l \rightarrow l + 1 \).
   3.3 multiply wavefunction by $r$ and normalize

Code Output to Experimental Observables

- each realization of the QTraj algorithm is a *quantum trajectory*
- average of $N$ quantum trajectories tends toward the solution of the Lindblad equation as $N \to \infty$
- overlap of resulting average trajectory with eigenstates, e.g., $\Upsilon(1S)$, $\Upsilon(2S)$, etc., used to compute survival probability of that state
- after accounting for feed down of excited states, results can be compared to experiment
Medium Interaction

- medium evolution implemented using a 3 + 1D dissipative relativistic hydrodynamics code using a realistic equation of state fit to lattice QCD measurements

- approximately $7 - 9 \times 10^5$ physical trajectories
  - production point sampled in transverse plane using nuclear binary collision overlap profile $N_{AA}^{\text{bin}}(x, y, b)$, initial $p_T$ from an $E_T^{-4}$ spectrum, and $\phi$ uniformly in $[0, 2\pi)$
  - 50-100 quantum trajectories per physical trajectory
  - allows for extraction of differential obserables including $v_2$ and results as a function of transverse momentum $p_T$

- vacuum evolution from initialization at $t_0 = 0$ fm until initialization of interaction with medium at $t = 0.6$ fm and vacuum evolution for $T < T_f = 290$ MeV (NLO $E/T$) and $T < T_f = 250$ MeV (LO $E/T$)
**Figure:** $R_{AA}$ for the $\Upsilon(1S)$, $\Upsilon(2S)$, and $\Upsilon(3S)$ as a function of $N_{\text{part}}$. The left panel shows variation of $\hat{\kappa} \in \{\kappa_L(T), \kappa_C(T), \kappa_U(T)\}$ and the right panel shows variation of $\hat{\gamma}$ in the range $-3.5 \leq \hat{\gamma} \leq 0$. In both panels, the solid line corresponds to $\hat{\kappa} = \hat{\kappa}_C(T)$ and the best fit value of $\hat{\gamma} = -2.6$. NLO $E/T$; from JHEP 08 (2022) 303.
**Figure:** $R_{AA}$ for the $\Upsilon(1S)$, $\Upsilon(2S)$, and $\Upsilon(3S)$ as a function of $p_T$. NLO $E/T$; from JHEP 08 (2022) 303.
\[ v_2[\Upsilon(1S)] \] vs. Centrality

**Figure:** The elliptic flow \( v_2 \) of the \( \Upsilon(1S) \) as a function of centrality compared to experimental measurements. LO \( E/T \); from *Phys. Rev. D* 104 (2021) 9, 094049.
\[ v_2[\Upsilon(1S)] \text{ vs. } p_T \]

**Figure:** The elliptic flow \( v_2 \) of the \( \Upsilon(1S) \) as a function of \( p_T \) compared to experimental measurements. LO \( E/T \); from *Phys.Rev.D* 104 (2021) 9, 094049.
\(v_2[\Upsilon(2,3S)]\) vs. Centrality

**Figure:** The elliptic flow \(v_2\) of the \(\Upsilon(2S)\) and \(\Upsilon(3S)\) as a function of centrality compared to experimental measurements. LO \(E/T\); from Phys.Rev.D 104 (2021) 9, 094049.
## Experimental References

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<th>Plot</th>
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<td>$v_2[\Upsilon(1S)]$ vs. Centrality</td>
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Theory References

- derivation of master and Lindblad equations
  - Phys. Rev. D 96 (2017) 3, 034021
- extraction of $R_{AA}$ and $v_2$ using QTraj code
  - JHEP 05 (2021) 136
  - Phys. Rev. D 104 (2021) 9, 094049
  - JHEP 08 (2022) 303
- QTraj code
Conclusions and Outlook

- due to hierarchies of scale, system of in-medium bottomonium ideally described using EFT methods, specifically pNRQCD, and the OQS formalism
- evolution equation takes the form of a Lindblad equation
- computational methods necessary to solve the Lindblad equation and extract observables including $R_{AA}$ and $v_2$
- QTraj code implements the quantum trajectories algorithm to solve the Lindblad equation and extract $R_{AA}$ and $v_2$ as functions of $N_{\text{part}}$ and $p_T$
- results show good agreement with experimental data
- method and results are fully quantum, non abelian, and heavy quark number conserving; take into account dissociation and recombination; and depend only on the transport coefficients $\kappa$ and $\gamma$ the values of which we take from lattice data
Thank you!