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Efficiently simulating quarkonium's evolution beyond the dipole approximation

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Abstract. The open quantum system framework allows one to compute quarkonium's evolution in a medium, keeping track of the needed quantum features. However, computing this evolution is a computationally demanding task. QTRAJ is an efficient code that allows one to simulate the behavior of quarkonium in a medium in the case in which the medium sees quarkonium as a small color dipole $rT \ll 1$. While this limit is accurate for $\Upsilon(1S)$, its applicability to other quarkonium states is unclear. In this talk, we present a generalization of this code that incorporates the regime where $rT \sim 1$ in the one-gluon exchange approximation. In its new version, QTRAJ implements new jump operators connecting different states, which are then expanded in plane waves, giving rise to a variation of the algorithm present in QTRAJ 1.0 where jumps with $\Delta\ell > 1$ are allowed. We will show a review of this approach comparing the $rT \ll 1$ and $rT \sim 1$ cases, and we present preliminary phenomenological results.

1 Introduction

The dynamics underlying the interactions between quarks and gluons in the quark–gluon plasma (QGP) generated in heavy-ion collisions (HIC) remain unclear from a theoretical perspective. At low baryochemical potential, the system undergoes a crossover phase transition, where the relevant degrees of freedom shift from hadrons to partons without a discontinuity in the order parameter. Nonetheless, certain bound states, such as quarkonia, are not fully incorporated into the hot bulk. Quarkonia are heavy quark-antiquark mesons, with constituent quark masses satisfying $m_Q \gg \Lambda_{QCD}$. They form colour-neutral pairs with very small radii. The combination of colourlessness and compact size makes quarkonia difficult to probe by the asymptotically free gluons of the medium. These properties are key to the survival of quarkonia in the thermal medium, although they are not completely shielded from interactions, and consequently not all quarkonia persist.

The partial dissociation of quarkonium was first studied under the framework of screened Coulombic-like potentials. The strategy was to use a Yukawa-like potential with an exponential dependence on a thermal *Debye mass*, that at leading order can be defined as:

$$m_D^2 = g^2 \left(\frac{2N_c + N_f}{6} \right) T^2 + O(g^3). \quad (1)$$

Despite some initial enthusiasm, experimental and lattice data point in a different direction, considering this effects just a partial answer for the suppression. Interest shifted then to dynamical approaches: collisions, interactions between the $Q\overline{Q}$ system and the gluons from the medium appear to contribute both in the dissociation and regeneration of quarkonia. An

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adequate treatment of this effects together can be achieved by an Open Quantum System (OQS) approach. The main idea consists of integrating out (tracing out in matrix terminology) the degrees of freedom of the environment [1] from the whole system evolution equation, and obtaining in exchange an evolution equation for the subsystem (quarkonia). Hence, the starting point is tracing the environment out from the Liouville-von Neumann equation:

$$\frac{d\rho_T}{dt} = -i[H_T, \rho_T] \quad \Longrightarrow \quad \mathrm{tr}_E\{\rho_T\} = \rho_Q \quad \Longrightarrow \quad \frac{d\rho_Q}{dt} = \mathrm{tr}_E\{-i[H_T, \rho_T]\}. \tag{2}$$

If we additionally perform the Born (weak coupling), Markov (absence of memory) and Born-Oppenheimer approximations (decoupled interactions between heavy and light degrees of freedom) we obtain the Lindblad equation:

$$\frac{d\rho_Q}{dt} = -i[H'_Q, \rho_Q] + \sum_{i=0}^{2} \int \frac{d^3q}{(2\pi)^3} \left(C_{i,\boldsymbol{q}} \rho_Q C^\dagger_{i,\boldsymbol{q}} - \frac{1}{2}\{C^\dagger_{i,\boldsymbol{q}} C_{i,\boldsymbol{q}}, \rho_Q\} \right), \tag{3}$$

where i is the color colour channel and q is the linear impulse transmitted by the virtual gluon. The **collapse operators** in our present work, extracted by applying the Hard Thermal Loop approximation while explicitly avoiding the multipole expansion in order not to be strictly limited to the dipolar regime, are given by:

$$C_{0,\boldsymbol{q}} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2N_c}} \\ \sqrt{C_F} & 0 \end{pmatrix} L_{\boldsymbol{q}}, \quad C_{1,\boldsymbol{q}} = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\frac{N_c^2-4}{4N_c}} \end{pmatrix} L_{\boldsymbol{q}}, \quad C_{2,\boldsymbol{q}} = \begin{pmatrix} 0 & 0 \\ 0 & \sqrt{\frac{N_c}{4}} \end{pmatrix} \bar{L}_{\boldsymbol{q}}, \tag{4}$$

where

$$L_{\boldsymbol{q}} = L^\dagger_{\boldsymbol{q}} \equiv 2g\sqrt{\Delta^<(q)}\,\sin\frac{\boldsymbol{q}\hat{\boldsymbol{r}}}{2}, \quad \bar{L}_{\boldsymbol{q}} = \bar{L}^\dagger_{\boldsymbol{q}} \equiv 2g\sqrt{\Delta^<(q)}\,\cos\frac{\boldsymbol{q}\hat{\boldsymbol{r}}}{2}. \tag{5}$$

We have assumed that only One-Gluon Exchange (OGE) [2, 3] interactions in Non-Relativistic QCD (NRQCD) are present. Also, we chose the Coulomb gauge. In turn, we obtained a dependence in the chromoelectric propagator $\Delta^<(q)$. Lastly, these last two matrix elements can be expanded in an spherical basis getting:

$$L_{\boldsymbol{q},t} = 8\pi g\sqrt{\Delta^<(q)}\,(-1)^t j_{2t+1}\left(\frac{qr}{2}\right) \sum_{m=-2t-1}^{2t+1} Y^m_{2t+1}(\Omega_{\boldsymbol{r}}) Y^{*m}_{2t+1}(\Omega_{\boldsymbol{q}}), \qquad \sum_{t=0}^{\infty} L_{\boldsymbol{q},t} = L_{\boldsymbol{q}}, \tag{6}$$

$$\bar{L}_{\boldsymbol{q},t} = 8\pi g\sqrt{\Delta^<(q)}\,(-1)^t j_{2t}\left(\frac{qr}{2}\right) \sum_{m=-2t}^{2t} Y^m_{2t}(\Omega_{\boldsymbol{r}}) Y^{*m}_{2t}(\Omega_{\boldsymbol{q}}), \qquad \sum_{t=0}^{\infty} \bar{L}_{\boldsymbol{q},t} = \bar{L}_{\boldsymbol{q}}. \tag{7}$$

2 QTRAJ and the Quantum Trajectories Algorithm

The framework of QTRAJ 1.0 [4] was created to simulate the propagation of individual quark pairs interacting in a medium by solving a Schrödinger equation with a effective Hamiltonian that is randomly interrupted by some stochastic jumps (transitions between well-defined angular momentum-color eigenstates). To recover physical results, we average over many trajectories as if we were computing an ensemble average. The effective hamiltonian:

$$H_{\mathrm{eff}} = H_Q - i\frac{\Gamma}{2} = H_Q - \frac{i}{2}\sum_n \int_{\boldsymbol{q}} C^\dagger_{n,\boldsymbol{q}} C_{n,\boldsymbol{q}} \tag{8}$$

will make the norm of the state decrease due to its non-Hermiticity. The non-Hermitian component of the Hamiltonian contains the decay width $-i\Gamma/2$ [5, 6], manifesting the inelastic

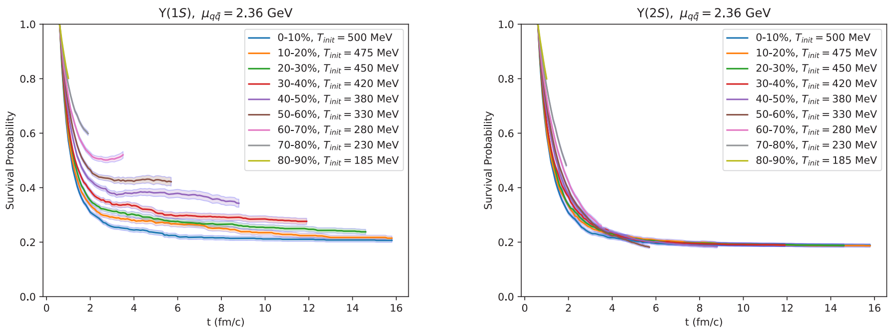

Figure 1. Normalized survival probability with respect to time for $\Upsilon(1S)$ and $\Upsilon(2S)$ (as Cornell eigenstates) from an initial S-wave gaussian (delta-like) pulse with $\sqrt{\langle r^2 \rangle} \approx 0.03$ fm.

collisions between the subsystem (quarkonium) and the environment (the QGP). If the initial state has been properly normalized, we can generate a random number $r_0 \in [0, 1]$ and once the norm of the state becomes smaller than r_0, the deterministic Schrödinger-like evolution is halted. We say then that a jump has been triggered, or in other words, that a gluon has interacted with our system. At this point, the stochastic evolution starts.

The stochastic evolution consists of projecting the current state with one specific collapse operator. In order to do so, we have to infer the values of the parameters final state it has been promoted. This is the **Quantum Trajectories** method [7, 8]. So we have to find the i, q, t and ℓ to project our vector state into:

$$\frac{C_{i,q,t,l' \to l} |\Psi\rangle}{\sqrt{\langle \Psi | \Gamma_{i,q,t,l' \to l} | \Psi \rangle}} \tag{9}$$

Here i labels which operator in eqs. (4) is responsible for the transition; q denotes the linear impulse transferred by the gluon to the pair; t is defined from eqs. (6) and (7); and ℓ is the angular momentum of the final state. The probability to get into a specific final state can be thought as:

$$p(q, c, t, \ell_f,) = p(c \cap q \cap t \cap \ell_f) = \underbrace{p(c|\Gamma)}_{r_1} \cdot \underbrace{p(q|\Gamma, c)}_{r_2} \cdot \underbrace{p(t|\Gamma, c, q)}_{r_3} \cdot \underbrace{p(\ell_f|\Gamma, c, q, t)}_{r_4} . \tag{10}$$

Every factor in eq. (10) can be regarded as a random draw from a probability distribution. Our work consists of an update that introduces these in the existing code, named QTRAJ 1.1 [9], and then the retrieval of some observables from a toy model in order to verify the qualitative features of the simulation and its feasibility as an instrument for phenomenological predictions.

3 Numerical results

We have divided the executions into 10 centrality classes, each of them associated with an uniform initial temperature in MeV, associated in turn to the entropy density of two overlapping nuclei within the Glauber optical model. 30,000 trajectories per centrality class have been then computed whose results are summed up in fig. 1 for the survival probability of

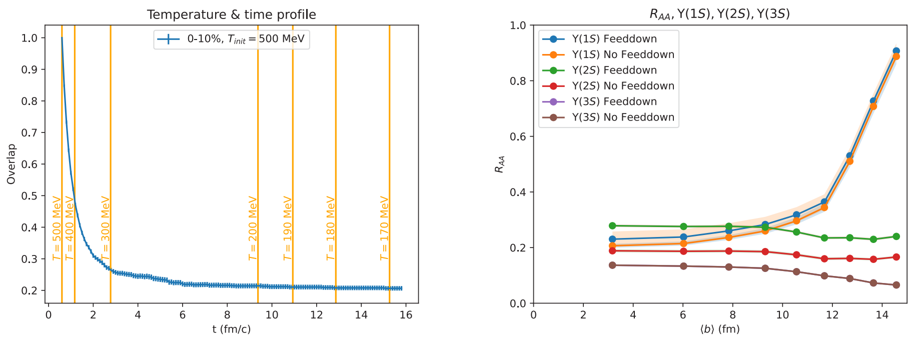

Figure 2. Profile of the population of 1S states for 0-10% centrality class and temperature thresholds associated (left). Nuclear modification factor R_{AA} as a function of the impact parameter b in fm for the lowest-energy S-waves of bottomonium (right). Υ(3S) is not enhanced because it is the highest energy state considered.

$\Upsilon(1S)$ and $\Upsilon(2S)$ for a narrow gaussian as an initial condition with $\sqrt{r^2} \approx 0.03$ fm and assuming Bjorken flow expansion. The size of the simulation box has been explicitly tested to avoid any border effects; however, the formalism does not include terms that lead to physical thermalization. Further work is being done to explicitly include these effects.

3.1 R_{AA} and feeddown

The nuclear modification factor is our target observable. It is defined as the ratio of an observable per nucleon in an AA collision versus a pp collision (in this case, detections of quarkonium per nucleon per unit of an interest variable X):

$$R_{AA}^{Q\overline{Q}}(p_\perp, y) = \frac{1}{\langle N_{coll}\rangle} \frac{\left(dN^{Q\overline{Q}}/dX\right)_{AA}}{\left(dN^{Q\overline{Q}}/dX\right)_{pp}} \tag{11}$$

In the right panel of fig. 2 we show the values of $R_{AA}^{Q\overline{Q}}$ as a function of the impact parameter b, corresponding to the centrality classes introduced in the previous section. Values smaller than unity, as those seen in the plot, indicate suppression. For our toy model, we are working under the assumption that no strong dissociation happens in pp collisions and that the expansion is purely governed by Bjorken flow. The plot illustrates how this mechanism scales for an increasing number of participant nucleons once the system emerges from the thermal medium. Additionally, to the plain output of QTRAJ 1.1, some feeddown has been included, although it only slightly enhances the quarkonium survival.

4 Conclusions

The implementation of QTRAJ 1.1 has been completed, and its qualitative descriptive power has been tested. We verified that, even with a non-tuned initial condition (delta-like 1S Gaussian), the survival probability approaches a stable asymptotic value. Moreover, the functional dependence of the $R_{AA}^{Q\overline{Q}}$ appears consistent with a stronger suppression of the $\Upsilon(1S)$ state for central collisions, which dominates the overlap with the initial wavefunction. On the other hand, much weaker suppression is observed in peripheral, which barely exceeds the deconfinement threshold.

The natural next step is to investigate the role of the initial distribution of $Q\overline{Q}$ pairs, specifically in terms of initial colour configuration, width, and angular momentum.

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