Efficiently simulating quarkonium's evolution beyond the dipole approximation

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Work done in collaboration with Andrea Beraudo, Paolo Parotto and Jorge Manuel Martínez Vera.

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- Heavy quarks can only be created at the beginning of the collision. It is a hard process.
- However, the existence of a medium changes the probability that a bound state is formed and its lifetime.
- Measuring R_{AA}, the ratio of quarkonium states measured in heavy-ion collisions divided by the naive extrapolation of pp data, we can extract information about the medium.

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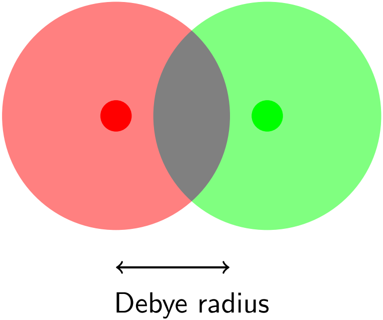
$$V(r) = -\alpha_s \frac{e^{-m_D r}}{r}$$

At finite temperature



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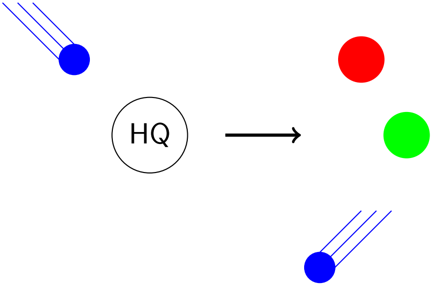
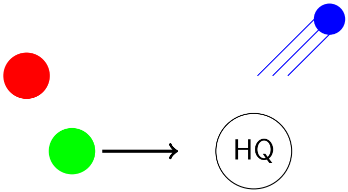


Recombination



Two heavy quarks coming from different origin may recombine to form a new quarkonium state.

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- When studying screening, we need to know if for a given potential a bound state solution exists. We need quantum mechanics to describe this.
- In some cases, decays and recombination can be described with rate or Boltzmann equation in the semi-classical approximation. However, this is not always the case.
- When thermal effects are important, we need to describe all three effects taking into account quantum effects.

Quarkonium as an Open quantum system

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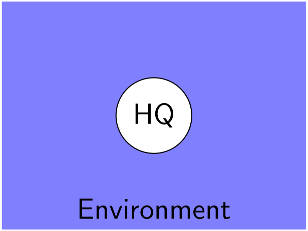

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- We can recover the Schrödinger equation and the Boltzmann equation as limits of the master equation in specific regimes.
- We need to derive the master equation from QCD. This has been done in:
  - Perturbation theory. Akamatsu (2015,2020), Blaizot and Escobedo (2017,2018).
  - Potential non-relativistic QCD (pNRQCD) in the $\frac{1}{r} \gg T$ regime. Brambilla et al. (2016,2017).
  - Schrödinger-Langevin equation (Gossiaux and Katz, 2016)

The Lindblad equation

Any master equation that is:

- Markovian
- Preserves the properties that a density matrix must fulfil (Hermitian, positive semi-definite, trace is conserve).

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In the case of quarkonium, the Markovian limit corresponds to the case in which the energy of the particles in the environment is larger than the binding energy.

Problems of the Lindblad equation

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- *Computational cost*. Since the state of the system is represented by a density matrix, if we use a lattice with the double of points, the cost is multiplied by four.
- *Black box*. From the Lindblad equation it is difficult to get a physical picture of what is the leading effect.
- *Solution*. Use the Quantum Trajectories method (Dalibard, Castin and Molmer, 1992). Monte Carlo technique to solve the Lindblad equation using wave functions instead of the density matrix.

The Monte-Carlo Wave Function method

Take the Lindblad equation

$$\partial_t \rho = -i[H(\gamma), \rho] + \sum_k \left(C_k(\kappa) \rho C_k^\dagger(\kappa) - \frac{1}{2} \{ C_k^\dagger(\kappa) C_k(\kappa), \rho \} \right)$$

Let us define

$$\Gamma_n = C_n^\dagger C_n \qquad \Gamma = \sum_n \Gamma_n$$

and

$$H_{eff} = H - i\frac{\Gamma}{2}$$

$\rho(t) = \sum_n p_n |\Psi_n(t)\rangle\langle\Psi_n(t)|$. If we know how to evolve the case $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$, it is straightforward to generalize.

The Monte-Carlo Wave Function method

The algorithm to evolve from t to $t + dt$

- With probability $1 - \langle\Psi(t)|\Gamma|\Psi(t)\rangle dt$.
  - Evolve the wave-function with $(1 - iH_{eff}\,dt)|\Psi(t)\rangle$. In our case, this implies solving a 1D Schrödinger equation because H_{eff} does not mix states with different color or angular momentum.
- With probability $\langle\Psi(t)|\Gamma_n|\Psi(t)\rangle dt$.
  - Take a quantum jump, $|\Psi(t)\rangle \to C_n|\Psi(t)\rangle$.
  - Only here transitions between different color and angular momentum are allowed.
- Normalize the resulting wave-function.

The average of this stochastic evolution of the wave-function is equivalent to the Lindblad equation for the density matrix.

How does the quantum trajectory method encode each effect?

- Screening. Through the Hermitian part of the Hamiltonian. If there are no bound states the heavy quark and antiquark will separate.
- Decay width. Through the Non-hermitian part of the Hamiltonian. Possibility to take a quantum jump to an unbound state.
- Recombination. Through jump operator. Finite probability to jump back to a bound state.

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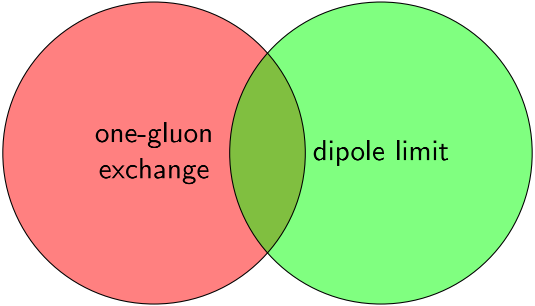
- This is a good approximation for bottomonium at the temperatures reached in current heavy-ion collisions, but not for charmonium.
- Goal: go beyond the dipole approximation in an efficient way.

Outline

Motivation

We wish to be able to efficiently simulate a larger set of possible master equations. Better description of charmonium and excited states.



We take the HTL one-gluon exchange case (Blaizot and Escobedo, 2018). However, the framework would be easily adapted to any one-gluon exchange model.

The master equation

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

where

$$H'_Q \equiv \begin{pmatrix} H'_s & 0 \\ 0 & H'_o \end{pmatrix} \equiv \begin{pmatrix} -C_F\dfrac{\alpha_s}{r}e^{-m_D r} & 0 \\ 0 & \dfrac{1}{2N_c}\dfrac{\alpha_s}{r}e^{-m_D r} \end{pmatrix}$$

Note also that the are infinitely many jump operators.

The master equation

Collapse operators

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where

$$C_q^0 \equiv \begin{pmatrix} 0 & \frac{1}{\sqrt{2N_c}} L_q \\ \sqrt{C_F} L_q & 0 \end{pmatrix} \quad C_q^1 \equiv \sqrt{\frac{N_c^2-4}{4N_c}}\begin{pmatrix} 0 & 0 \\ 0 & L_q \end{pmatrix}$$

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where

$$L_q \equiv g\sqrt{\Delta^>(\omega=0,q)} S_{\mathbf{q}\cdot\mathbf{r}} \quad \text{and} \quad \overline{L}_q \equiv g\sqrt{\Delta^>(\omega=0,q)} C_{\mathbf{q}\cdot\mathbf{r}}$$

and $\Delta^> = \langle A_0 A_0 \rangle$ in the HTL approximation, $S_{\mathbf{qr}} = 2\sin\left(\frac{\mathbf{qr}}{2}\right)$ and $C_{\mathbf{qr}} = 2\cos\left(\frac{\mathbf{qr}}{2}\right)$.

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Approach

$$S_{\mathbf{qr}} = 2\sin\left(\frac{\mathbf{qr}}{2}\right) = -i\left(\mathrm{e}^{i\frac{\mathbf{qr}}{2}} - \mathrm{e}^{-i\frac{\mathbf{qr}}{2}}\right)$$

and then we can make use of the identity

$$\mathrm{e}^{i\mathbf{kr}} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l j_l(kr) Y_l^m(\Omega_k) Y_l^{m*}(\Omega_r)$$

Rewriting the Lindblad equation

$$\int \frac{d^3q}{(2\pi)^3} \to \int_0^\infty dqq^2 \sum_{t=0}^{\infty} \sum_m$$

$$L_{\mathbf{q}} \to g\sqrt{\frac{2\Delta^>(0,q)}{\pi}} j_{2t+1}\left(\frac{qr}{2}\right) Y_{2t+1}^m(\Omega_r)$$

and

$$\overline{L}_{\mathbf{q}} \to g\sqrt{\frac{2\Delta^>(0,q)}{\pi}} j_{2t}\left(\frac{qr}{2}\right) Y_{2t}^m(\Omega_r)$$

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Equivalent

Same physics. We just trade a 3-D parameter $\mathbf{q}$ by a continous parameter q and two discrite ones (t and m).

Example. Plane wave expansion of Laine's potential

$$\mathrm{Im}\, V_s(r) = -\frac{g^2 C_F}{8\pi^2}\int_0^\infty dq q^2 \Delta^>(0,q)\left(1-\frac{\sin(qr)}{qr}\right) =$$

$$= -\frac{g^2 C_F}{4\pi^2}\sum_{t=0}^\infty (4t+3)\int_0^\infty dq q^2 \Delta^>(0,q)\left(j_{2t+1}\left(\frac{qr}{2}\right)\right)^2$$

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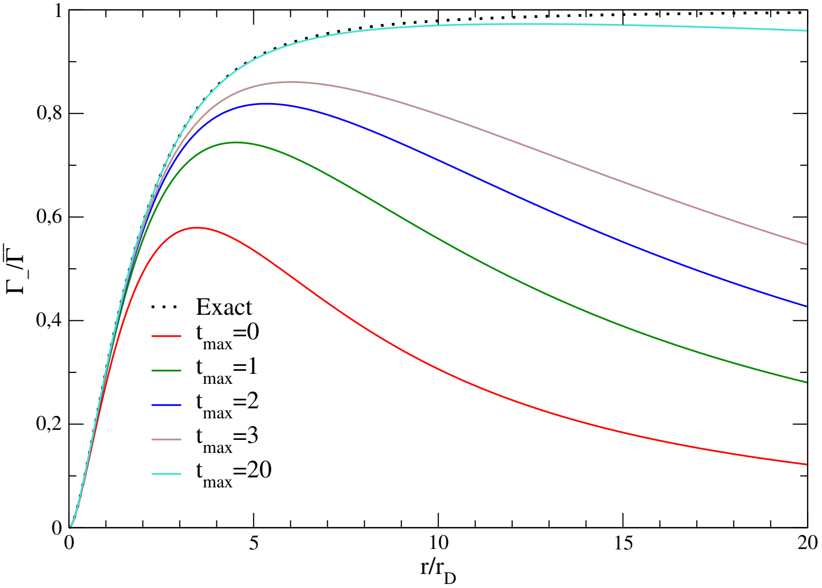
Cross-check

Can be also shown to be true using the following identities from Abramowitz and Stegun

$$\sum_{n=0}^{\infty} (2n+1)(j_n(z))^2 = 1 \quad \sum_{n=0}^{\infty} (-1)^n (2n+1)(j_n(z))^2 = \frac{\sin(2z)}{2z}$$

t expansion of Laine's potential



Structure of a jump

A jump is parametrized by the parameters of the corresponding jump operator producing it plus the out-going angular momentum

$$P_{jump}(i, q, t, l)$$

To simplify the implementation of the code, we can think of it in the following way

$$P(i)P(q|i)P(t|q,i)P(l|t,q,i)$$

$P(i)$

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- An octet can either go to a singlet ($i = 0$) or to an octet ($i = 1$ or $i = 2$).
- $\Gamma_o = \sum_{i=0}^{2} \Gamma_o^i$. We generate a random number x between 0 and 1.
  - If $x < \frac{\langle\Psi|\Gamma_o^0|\Psi\rangle}{\langle\Psi|\Gamma_o|\Psi\rangle}$, then $i = 0$.
  - Elseif $x < \frac{\langle\Psi|\Gamma_o^0+\Gamma_0^1|\Psi\rangle}{\langle\Psi|\Gamma_o|\Psi\rangle}$, then $i = 1$.
  - Else, $i = 2$.

Example: $P_s(q|0)$

$$P_s(q|0) = \frac{\frac{g^2 C_F}{4\pi^2} q^2 \Delta^{>}(0,q) \langle \Psi | 1 - \frac{\sin(qr)}{qr} | \Psi \rangle}{\langle \Psi | \Gamma_s | \Psi \rangle}$$

Probability distribution. We can get random values of q following this distribution using standard techniques. For example, we use the accept-reject method.
However, this is slow. We can do better by understanding this distribution as a 2D distribution for q and r. Using accept-reject we can get q and r values. Then, we take only the q value.

$P(t|q_c, 0)$

$$P(t|q_c,0)=(4t+3)\frac{\langle\Psi|\left(j_{2t+1}\left(\frac{q_c r}{2}\right)\right)^2|\Psi\rangle}{2\langle\Psi|1-\frac{\sin(q_c r)}{q_c r}|\Psi\rangle}$$

Similarly to $P(i)$, we can decide which t is taken generating a random number.

Orbital angular momentum

Once we know t, we know that the jump operator is going to act with Y^m_{2t+1}. Using the Wigner-Eckart theorem, we can prove that

$$\sum_{m,m'} Y^m_{2t+1}|l'm'\rangle\langle l'm'|Y^{m*}_{2t+1} = \sum_{m''} p_{l'\to l}|lm''\rangle\langle lm''|$$

$p_{l'\to l}$ is a probability that can be computed using Crebsch-Gordon coefficients.

$$p_{l'\to l} = |\langle l,0;2t+1,0|l',0\rangle|^2$$

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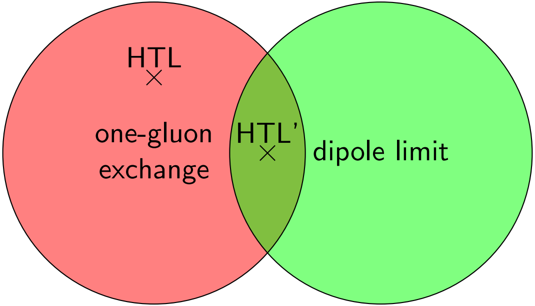
- However, there is a subtlety. The dipole limit means that $\frac{1}{r} \gg T, m_D \gg E$. The HTL master equation we are using works in the regime $T \gg \frac{1}{r} \sim m_D$.
- These two regimes are not connected. We would need to go throught the regime $\frac{1}{r} \sim T \gg m_D$.

Mapping the issue



We need to propose a new master equation (HTL') that can be modeled with both versions of *Qtraj*. It doesn't need to represent any physical situation.

HTL in the $rm_D \ll 1$ limit

The naive expansion

$$\Gamma_s(\hat{r}) = \frac{g^2 C_F}{2\pi^2} \int dq q^2 \Delta^<(q) \left(1 - \frac{\sin(q\hat{r})}{q\hat{r}}\right)$$

If we expand naively for small r

$$\Gamma_s(\hat{r}) \approx \frac{g^2 C_F \hat{r}^2}{12\pi^2} \int dq q^4 \Delta^<(q)$$

However, the integral diverges in the UV. This is because the HTL approximation is not valid for large q. However, taking the full one-loop $\Delta^<(q)$ in thermal field theory would be too complicated for our purposes.

HTL in the $rm_D \ll 1$ limit

Integration by regions

We can split the integral in two regions. Regulate each piece in dimensional regularization and then add them. One regions is $q \sim m_D$ and the other $q \sim \frac{1}{r}$.

$$\Gamma_s(\hat{r}) = \kappa(\hat{r})\hat{r}^2$$

with

$$\kappa(\hat{r}) = \alpha_s C_F \frac{m_D^2 T}{6}\left[\frac{1}{3}(4 - 3\gamma_E - 3\log 2) - \log\left(\frac{m_D \hat{r}}{2}\right)\right]$$

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- The answer is no.

The modified HTL

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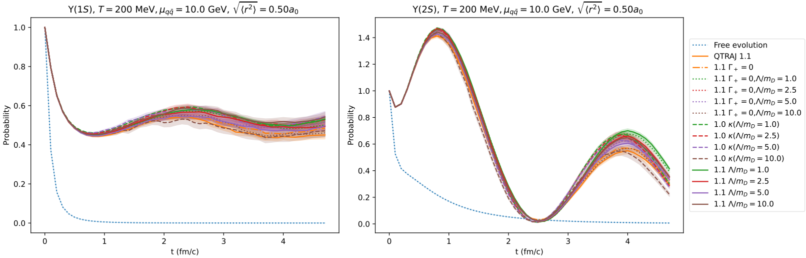
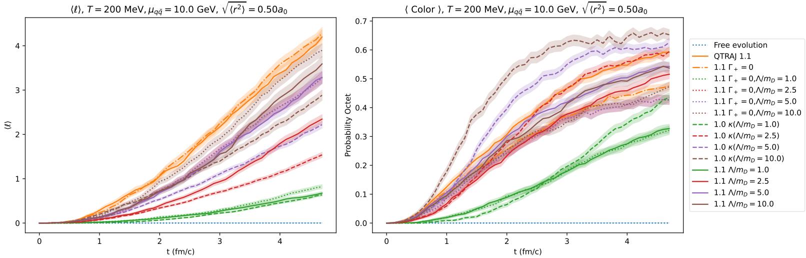
Comparison of both versions of *Qtraj*

Survival probability at constant temperature.



Comparison of both versions of *Qtraj*

Average orbital momentum and color.



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- The code is working as expected.

Outline

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- We are working on phenomenological results using the new version of *Qtraj*.

Thank you for your attention

Questions?