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Full Length Article

Towards an optimally sensitive temperature probe in heavy-ion collisions

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ABSTRACT

The high-precision heavy quarkonium data from LHC Run 2 and the ongoing Run 3 provide a unique window into the properties of hot nuclear matter and the Quark-Gluon Plasma (QGP). To make full use of this data, it is crucial to go beyond traditional observables such as the nuclear modification factor R_{AA} and elliptic flow v_2, and instead develop new probes that are more directly sensitive to the characteristics of the medium.

We adopt the open quantum systems perspective for in-medium quarkonium and take inspiration from cold atom metrology techniques to construct observables with optimal sensitivity to specific QGP parameters. Focusing on the bulk temperature, we develop such optimal observables based on the Caldeira-Leggett master equation as a simplified setup, with the goal of extending it to a full Quantum Brownian Motion Lindblad equation.

1. Impurities as key observables

In the analysis of the properties of the QGP, the hard probes, such as jets and heavy quarkonia, are among the most popular observables. These phenomena can be regarded as impurities of the plasma and are useful because they interact with the environment enough to carry information, but their properties survive the freeze-out so they can be detected.

In this context, a heavy quark impurity in the QGP is not that different from a heavy atom impurity in a Bose-Einstein condensate (BEC) [1], so it is possible to use in the study of heavy-ion collisions tools that are well established in the study of cold atoms.

This work consists of a brief introduction of the topic applied to quarkonium inside the QGP, as well as the proposal of a general method that can be used to obtain new observables in heavy-ion collisions. Finally, a proof-of-principle on a much simpler setup to demonstrate the applicability of the method is presented. The standard $\hbar = c = k_B = 1$ convention is used except when indicated otherwise.

1.1. Quarkonium as a probe for the quark-gluon plasma

In the past, the interactions of quarkonium states, as probes of the QGP, with their environment were mainly studied through simple potential models. With the maturation of effective field theory methods (such as non-relativistic QCD and potential non-relativistic QCD (NRQCD and pNRQCD)) at finite temperature T, the concept of a potential was put on a conceptually rigorous footing and it was found that the in-medium interaction potential between heavy quarks is complex (for a review see [2]). Subsequently, the static picture of in-medium quarkonium, based e.g. on the concept of melting temperatures (the QGP thermometer [3]), gave way to a dynamical picture in terms of decoherence of the quantum wavefunction [4].

1.2. Open quantum systems approach

The Open Quantum Systems (OQS) formalism provides a unified language to describe the dynamics of small probe systems coupled to an environment. Making heavy use of separation of scales, it aligns well with the effective field theory description of quarkonium and various OQS formulations have been derived based on NRQCD and pNRQCD [2,4–6].

The Hamiltonian of a system where a quantum state (the probe) is weakly coupled to a thermal medium (the bath) can be written as

$$\hat{H}_{\mathrm{T}} = \hat{H} \otimes \hat{I}_{\mathrm{B}} + \hat{I} \otimes \hat{H}_{\mathrm{B}} + \hat{H}_{\mathrm{int}} \, , \tag{1}$$

where the subscript B denotes the bath, absence of a subscript indicates the probe and $\hat{H}_{\mathrm{int}}$ is the interaction Hamiltonian.

The evolution of the density matrix of the whole system $\hat{\rho}_{\mathrm{T}}$ is given by the von Neumann [7]:

$$\frac{d\hat{\rho}_{\mathrm{T}}}{dt} = -i[\hat{H}_{\mathrm{T}}, \hat{\rho}_{\mathrm{T}}]. \tag{2}$$

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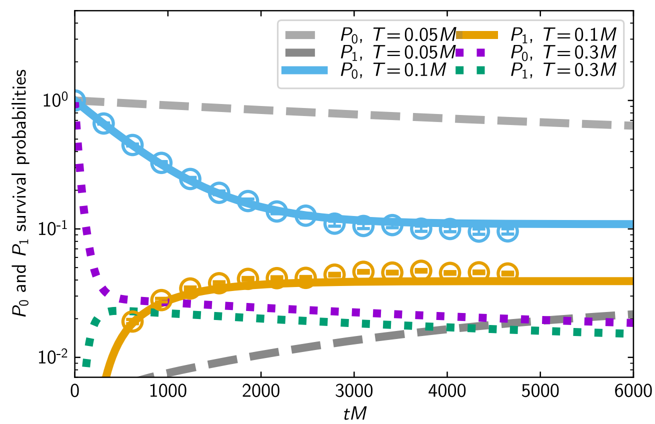

Fig. 1. Survival probabilities of the ground and first excited states against dimensionless scaled time tM, where M is an arbitrary mass scale, via the direct solution of the master equation (3) for the 1D case on a 248^2 grid at $T = 0.1M$ (solid lines) compared with the approximate solution via the stochastic quantum state diffusion unraveling (open circles), and full Lindblad dynamics for $T = 0.05M$ and $T = 0.3M$ (dashed and dotted lines, respectively). Figure reproduced from [6] using the code from [8].

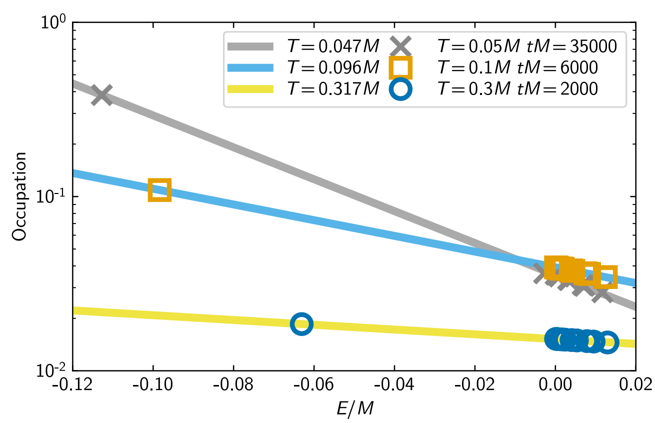

Fig. 2. Occupation versus the dimensionless scaled energy of the individual states (data points) in the one-dimensional case on a 248^2 grid. The solid lines represent the fit to a Boltzmann distribution where it is clear that the probe thermalizes and the fitted temperature approaches to the temperature of the environment. Figure reproduced from [6] using the code from [8].

To obtain the density matrix of the probe from the total density matrix it is just necessary to trace out the degrees of freedom of the bath, $\hat{\rho} = \mathrm{Tr}_B[\hat{\rho}_T]$.

The obtained evolution of the probe density matrix is equivalent to the solution of the appropriate Lindblad equation [7]:

$$\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}] + \sum_k \gamma_k \left(\hat{L}_k \hat{\rho} \hat{L}_k^\dagger - \frac{1}{2}\{\hat{L}_k^\dagger \hat{L}_k, \hat{\rho}\} \right), \tag{3}$$

where the Hamiltonian is the Hamiltonian of the probe and the so-called jump operators, $\hat{L}_k$, can be obtained from the interaction Hamiltonian. γ_k are a set of non-negative real coefficients called damping rates. The Lindblad equation ensures all the good properties of the density matrix are preserved throughout the evolution: positivity ($\langle n|\hat{\rho}|n\rangle > 0$) and hermiticity ($\hat{\rho}^\dagger = \hat{\rho}$) are guaranteed as well as the fact that the trace of the density matrix remains one ($\mathrm{Tr}[\hat{\rho}] = 1$).

1.2.1. 1+1D Quarkonium evolution

The evolution of one-dimensional quarkonium has been successfully reproduced numerically in [6]. The survival probabilities match the approximation given by quantum state diffusion as seen in Fig. 1. The thermalization of the states can also be seen in Fig. 2 where the fit to a Boltzmann distribution ($\propto e^{-E/T}$) gives the temperature expected from the medium interaction.

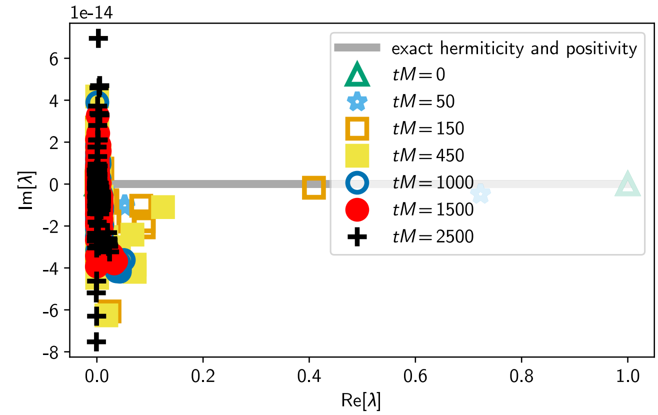

Fig. 3. Location on the complex plane of the eigenvalues of the density matrix in the 3D case on an 8^6 grid. All the eigenvalues are located in the real axis up to numerical error (the scale on the imaginary part is given in units of 10^{-14}). Code available at [9].

1.2.2. 3+1D Quarkonium evolution

Meanwhile, in the 3D case, the code has been successfully implemented [9], but it is limited by the available computational resources. The numerical approach requires space discretization into n possible position, which makes the density matrix a $n^{2d} \times n^{2d}$ matrix with $d = 3$, the number of dimensions. Thus, phenomena like thermalization is really difficult to realize due to the small grid size. The challenge now is to finalize the ongoing memory optimization on [9] to allow the code to be useful on bigger grid sizes.

Nevertheless, the "good properties" of the density matrix are still preserved. The positivity and hermiticity preservation can be seen in Fig. 3.

2. Quantum metrology

Quantum metrology allows the highest possible precision in the estimation of physical parameters, surpassing even classical limits [10]. In the case of measuring, e.g. the temperature of a system, the uncertainty in the estimation of the temperature from the measurement of some observable $\hat{A}$ through repeated measurements on independent identical preparations is given by [1]:

$$\delta T[\hat{A}] = \sqrt{\frac{\langle \hat{A}^2\rangle - \langle \hat{A}\rangle^2}{N\chi_T^2[\hat{A}]}} \tag{4}$$

where the temperature susceptibility of the observable is $\chi_T[\hat{A}] = \partial_T \mathrm{Tr}[\hat{\rho}\hat{A}]$ and N is the sample size (number of independent measurements).

Then, it is useful to define the so-called symmetric logarithmic derivative (SLD) Λ_T through the generalized Lyapunov equation [11]:

$$\partial_T \hat{\rho}(T) = \frac{1}{2}\{\hat{\Lambda}_T, \hat{\rho}(T)\} - \hat{\rho}(T)\langle\hat{\Lambda}_T\rangle. \tag{5}$$

The SLD is the quantity that minimizes the uncertainty as expressed in (4), i.e. is the optimal observable, that saturates the Cramér-Rao inequality [12]. Thus, it can be used to compute the Quantum Fisher Information (QFI), $\mathcal{F}_T = \langle\hat{\Lambda}_T^2\rangle$, which is the maximum amount of information that can be extracted about a certain physical parameter (the temperature in this case) from a quantum system.

2.1. From the density matrix

In the literature, the estimation of the SLD (and the QFI by extension) is done through the knowledge *a priori* of the density matrix [1]. The

SLD can be decomposed into Hermitian operators (i.e. observables), e.g. different combinations of position and momentum operators, $\hat{x}$ and $\hat{p}$, respectively:

$$\hat{\Lambda} = c_x\hat{x} + c_p\hat{p} + c_{\{x,p\}}\{\hat{x},\hat{p}\} + c_{x^2}\hat{x}^2 + c_{p^2}\hat{p}^2 + \cdots = \sum_i c_i \hat{A}_i \ , \tag{6}$$

and then the c_i coefficients can be obtained from (5) if the explicit form of the density matrix is known.

Nevertheless, the density matrix is only known for few simple systems such as point particles. Furthermore, it is usually only known in the steady state, i.e. in the equilibrium, which makes impossible to use it to extract information about dynamical phenomena such as transport or energy loss.

2.2. From the master equation

However, even if the density matrix is not known explicitly, knowing the master equation is enough to determine the SLD [13]. In general, the master equation can have the following form:

$$\partial_t\hat{\rho}(t,T) = \mathcal{L}[T]\hat{\rho}(t,T) \ , \tag{7}$$

where $\mathcal{L}[T]$ is a linear superoperator acting on the density matrix that can depend on the temperature. The Schwarz's theorem can be used to identify the time derivative of (5) with the temperature derivative of the master equation (7):

$$\partial_t(\partial_T\hat{\rho}) = \partial_T(\partial_t\hat{\rho}) \ , \tag{8}$$

and, through the SLD decomposition (6), it is possible to obtain the c_i coefficients by projecting onto the observable basis $\{A_j\}$ and solving the corresponding system of equations [13]:

$$\mathrm{Tr}[\{\partial_t(\partial_T\hat{\rho}) - \partial_T(\partial_t\hat{\rho})\}\hat{A}_j] = 0. \tag{9}$$

This allows to obtain the SLD expression, and thus the QFI without solving the master equation, which is particularly useful when the density matrix is not known or it is very complicated to compute.

The goal now is to have a suitable model for the in-medium quarkonium evolution master equation [4,5] and apply this method to it using, e.g. spectrum operators as the basis of observables.

3. Proof of principle: Caldeira-Leggett master equation

However, instead of tackling directly the quarkonium master equation, the presented formalism can be verified using a simpler theoretical setup. Thus, we study the quantum Ornstein-Uhlenbeck motion, i.e. the Quantum Brownian Motion (QBM) with a harmonic potential [7]. In this model, the evolution of a heavy point particle impurity inside an Ohmic environment is given by the so-called Caldeira-Leggett master equation [7], where the $\hbar$ is recovered for clarity purposes:

$$\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar}[\hat{H},\hat{\rho}] - \frac{2m\gamma k_B T}{\hbar^2}[\hat{x},[\hat{x},\hat{\rho}]] - \frac{i\gamma}{\hbar}[\hat{x},\{\hat{p},\hat{\rho}\}] \ , \tag{10}$$

where the single particle Hamiltonian is:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}. \tag{11}$$

The explicit solution can be easily obtained on the steady state [7]:

$$\rho(x,x') = \frac{1}{\sqrt{2\pi\sigma_x^2}}\exp\left[-\frac{1}{2\sigma_x^2}\left(\frac{x+x'}{2}\right)^2 - \frac{\sigma_p^2}{2\hbar^2}(x-x')^2\right] \ , \tag{12}$$

where $\sigma_x^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ and $\sigma_p^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2$. This allowed in [1] to obtain the SLD for the temperature in this QBM setup as:

$$\hat{\Lambda}_T^{\mathrm{QBM}} = c_x^2(\hat{x}^2 - \langle\hat{x}^2\rangle) + c_p^2(\hat{p}^2 - \langle\hat{p}^2\rangle) \ , \tag{13}$$

where the coefficients:

$$c_{x^2} = \frac{4\langle\hat{p}^2\rangle^2\chi_T[\hat{x}^2] + \hbar^2\chi_T[\hat{p}^2]}{8\langle\hat{x}^2\rangle^2\langle\hat{p}^2\rangle^2 - \hbar^4/2} \ , \quad c_{p^2} = \frac{4\langle\hat{x}^2\rangle^2\chi_T[\hat{p}^2] + \hbar^2\chi_T[\hat{x}^2]}{8\langle\hat{x}^2\rangle^2\langle\hat{p}^2\rangle^2 - \hbar^4/2}. \tag{14}$$

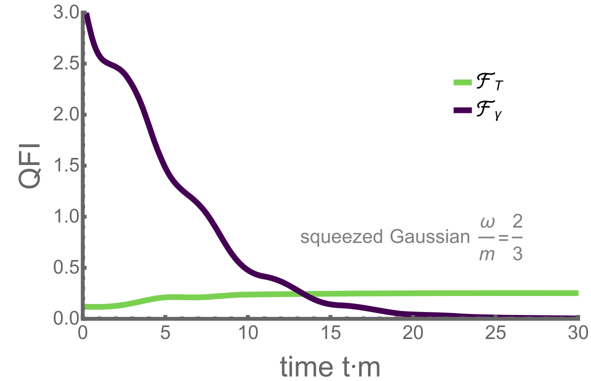

Fig. 4. The Quantum Fisher Information versus dimensionless scaled time. It is clear that the obtainable information from the decay rate quickly vanishes with time, which is expected from the fact that the steady state has no decay rate dependence. On the other side, the available information from the temperature is maintained at late times after having increased slightly from the early moments of the evolution, which indicates a thermalization of the probe with the bath. Figure extracted from [13].

As expected, the same solution can be achieved without the need of the explicit density matrix [13]. Moreover, the solution in the dynamical case can be computed and matches the complicated analytical expression [13].

One key feature of this approach is that it allows the study of the decay rate, γ, that appears in (10), and it is inaccessible from the steady solution. Thus, the decay rate SLD, Λ_γ, (and its QFI, $\mathcal{F}_\gamma$) can be created analogously and it is possible to obtain information from the decay rate and the transient regime by measuring the position and momentum spread on the early times (see Fig. 4).

4. Conclusions and outlook

Impurities have been established as a tool to study static and dynamic properties of the medium, and in that regard it has been shown that it is possible to use them to develop new observables. In the context of QCD, it has been discussed the issues of the study of quarkonium evolution inside the QGP and as well as the challenge of defining new observables.

The key idea behind defining new observables is using the OQS formalism to obtain the master equation and use this to get the SLD as a new measurable quantity. It also gives information about the maximum precision achievable in estimating certain parameters encoded in a quantum state through the QFI.

The analysis in the case of the QBM, described by the Caldeira-Leggett master equation, served as the ideal setup for a successful proof of principle on the applicability of the method. The remaining and the most important step is its application to the quarkonium master equation.

With a full OQS quarkonium description and the presented method, it is expected the development of new (and better) observables for the temperature (T), the screening mass (m_D), the color correlation length (ℓ), and even the specific shear viscosity (η/S) or the energy-loss ($\hat{q}$), among others.

CRediT authorship contribution statement

Víctor López-Pardo: Writing – original draft, Investigation, Conceptualization; **Alexander Rothkopf:** Supervision, Investigation, Conceptualization.

Data availability

No data was used for the research described in the article.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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