From Complex to Stochastic Potential: Heavy Quarkonia in the QGP

Alexander Rothkopf
Albert Einstein Center for Fundamental Physics
University of Bern

In collaboration with
Heavy Quarkonia: Physics Motivation

- Explore the physics of the phase transition at $T_C \approx 200$ MeV
- Hadronic thermometer: Heavy Quarkonia ($J/\Psi, \Upsilon$) (Matsui, Satz 1986)
Experiments do measure heavy quarkonium suppression at RHIC and LHC

- Large quark mass allows a separation of scales
  - Goal: Derive the potential from first principles QCD
- Need to develop fully dynamical models of QQ suppression
  - Goal: Treat effects at finite T consistently, e.g. spatial decoherence
Theoretical progress

- Goal is to derive a Hamiltonian with:

\[ H = \frac{p_1^2}{2m_Q} + \frac{p_2^2}{2m_Q} + V^{(0)}(R) + V^{(1)}(R) \frac{1}{m} + \ldots \]

- At \( T=0 \) systematic framework available: NRQCD, pNRQCD

  Brambilla et al. 2005

- Potential Models at \( T>0 \) Nadkarni, 1986

  Ad-hoc choice: Free Energies or Internal Energies

  No Schrödinger equation available, gauge dependent, handling of entropy?
Perturbative derivations of $V^0(R)$

Direct Calculation of the Wilson loop in Hard Thermal Loop PT

$W_{\square}(t, R) = \frac{gC_F}{4\pi} \left( m_D + \frac{e^{-m_D R}}{R} \right) - \frac{ig^2 TC_F}{4\pi} \phi(m_D R)$

$\phi(x) = \int_0^\infty dz \frac{z}{(z^2 + 1)^2} \left[ 1 - \frac{\sin[zx]}{zx} \right]$

Debye screening: a cloud of quarks and gluons mitigates the interaction effects
Landau damping: collisions with the deconfined environment

Effective field theory treatment using perturbation theory

- Treats explicitly all different scales in the system
- Additional contributions to real and imaginary part: e.g. Singlet to Octet brake-up

Question: How to obtain the potential non-perturbatively

Brambilla, Ghiglieri, Vairo and Petreczky PRD 78 (2008) 014017
A different viewpoint on Heavy Quarkonia

- Determine the spectra of heavy quarkonia directly from Lattice QCD

**LQCD: Monte Carlo**

Cannot measure spectral function directly

**Infer** from a measurable quantity instead:
Maximum Entropy Method

Judging the survival of $J/\psi$ through an inspection by eye

Task at hand: To combine the clarity of the potential picture with non-perturbative capabilities of lattice QCD
Overall strategy: Separation of scales

- Use only the following separation of scales

\[ \frac{\Lambda_{QCD}}{m_Q c^2} \ll 1, \quad \frac{T}{m_Q c^2} \ll 1, \quad \frac{p}{m_Q c} \ll 1 \]

- Select appropriate degrees of freedom

Relativistic thermal field theory \rightarrow Derivation of the heavy quark potential \rightarrow Quantum mechanics

- Obtain a dynamical Schrödinger equation with non-perturbative potential \( V^0(R) \)
A QQbar wavefunction

- Relativistic field theory: Meson Currents
  \[ J(x) = \bar{Q}(x) \Gamma Q(x) \]
- Test charges: introduce external separation
  \[ M(R, t) = \bar{Q}(x, t) \Gamma W(x, y, t) Q(y, t) \]
- Time evolution: Gauge invariant description
  \[ D^>(R, t) = \langle M(R, t) M^\dagger(R, 0) \rangle \]

- At T=0 rigorously defined as Nambu-Bethe-Salpeter wavefunction
  \[ \Psi_{\text{NBS}}(R, t) = \langle 0 | M(R, t) | Q \bar{Q} \rangle \]

- At T>0, attempt a generalization via the Mesic correlators
  \[ \Psi_{Q\bar{Q}}(R, t) \overset{\text{match}}{=} D^>(R, t) = \left\langle \mathcal{T} \left[ \int \mathcal{D}[\bar{Q}, Q] \Gamma \bar{W} W^\dagger Q(y') \bar{Q}(y) Q(x) \bar{Q}(x') e^{iS_{Q\bar{Q}}[Q, \bar{Q}, A]} \right] \right\rangle \]

Review: Aoki, Hatsuda, Ishii

Barchielli et. al. 1988
Iida, Ikeda PoS(Lat 2011)195

März 9, 2012
Three steps towards the potential

I. Integrate out rest energy: Foldy-Tani-Wouthuysen expansion in $1/mc^2$

$$S_{QQ}^{FTW}[\mathcal{A}] = \bar{Q}(x) \left[ \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} D_0 - mc + \frac{g}{2mc^2} \begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix} B^i + \frac{1}{2mc} D_i^2 \right] Q(x)$$

Upper and lower components decouple: Pauli Spinors $Q= (\chi, \xi)$ both contribute

II. Grassmann Integration: Replace pairs of $\chi \chi^\dagger$, $\xi \xi^\dagger$ with QM Green’s functions $S$

No fermion determinant since heavy quarks do not appear in virtual loops

$$D_{QM}^\gamma = \mathcal{T} \left[ W(x, y) G S(y, y') \bar{G} W^\dagger(x', y') S^\dagger(x, x') \right]$$

Temperature dependence 2x2 Matrix Spin Structure Quantum mechanical Greens function

III. Write greens functions as QM path integrals (quark propagation amplitude):

$$S(x, x') = \int_x^{x'} D[z, p] \mathcal{T} \exp \left[ i \int_t^{t'} dt \left( p(t) \dot{z}(t) - \frac{1}{2m} \left( p(t) - \frac{g}{c} A(z(t), t) \right)^2 - g A^0(z(t), t) + \frac{g}{mc} \sigma_i B^i(z(t), t) \right) \right]$$

Barchielli et. al. 1988
Defining the Heavy Quark Potential

- Combine the path integrals for each single quark/antiquark

\[
D_{QM}^> = \exp[-2imc^2t] \int D[z_1, p_1] \int D[z_2, p_2] \times \\
\exp \left[ i \int_t^{t'} ds \sum_i \left( p_i(s) \dot{z}_i(s) - \frac{p_i^2(s)}{2m} \right) \right] \left\langle \frac{1}{N} \text{Tr} \left[ \mathcal{P} \exp \left[ \frac{ig}{c} \oint_C dx^\mu A_\mu(x) \right] \right] \right\rangle
\]

- Use the transfer matrix to read off the Hamiltonian

\[
\langle \text{Tr} \left[ \exp \left[ \oint \mathbf{A} \right] \right] \rangle \equiv \exp \left[ i \int_t^{t'} ds \, U(z_1(s), z_2(s), p_1(s), p_2(s), s) \right]
\]

- Systematic expansion of the potential in p/mc

\[
i \log \left[ \langle W(z(t), t) \rangle \right] = \int_t^{t'} ds \left( V^0(z, s) \big|_{p=0} + V^1_{n,i}(z, s) \big|_{p=0} \frac{p_i(s)}{mc} + \ldots \right)
\]

- In the static limit: rectangular Wilson loop contour \( W_\square(R, t) \)

- Take the time derivative to obtain the potential \( V^0(R) \) at late \( t \)

\[
\lim_{t \to \infty} \frac{i \partial_t W_\square(R, t)}{W_\square(R, t)} = V^0(R)
\]
The Potential and Spectral Functions

Make time dependence of the Wilson loop explicit (here in real-time)

\[ W(R, t) = \int_{-\infty}^{\infty} d\omega \ e^{-i\omega t} \rho(R, \omega) \]

In the infinite mass limit: \( \rho(R, \omega) = \rho_{\square}(R, \omega) > 0 \)

\[ V^0(R) = \lim_{t \to \infty} \frac{\int_{-\infty}^{\infty} d\omega \ \omega \ e^{-i\omega t} \rho_{\square}(R, \omega)}{\int_{-\infty}^{\infty} d\omega \ e^{-i\omega t} \rho_{\square}(R, \omega)} \]

At each \( R \), lowest lying peak determines the potential

Two analytically solvable cases: Breit-Wigner and Gaussian

\[ \rho_{BW}(R, \omega) \propto \frac{\Gamma(R)}{\Gamma^2(R) + (\omega_0(R) - \omega)^2} \quad V_{BW}^0(R) = \omega_0(R) - i\Gamma(R) \]

\[ \rho_{G}(R, \omega) \propto \text{Exp} \left[ -\frac{(\omega_0(R) - \omega)^2}{2\Gamma^2(R)} \right] \quad V_{G}^0(R) = \omega_0(R) - i\Gamma^2(R)t \]
We can measure neither $\rho(R, \omega)$ nor $W_{\square}(R, t)$ directly in Lattice QCD

$W_{\square}(R, t) = \int_{-\infty}^{\infty} d\omega \, e^{-i\omega t} \rho_{\square}(R, \omega)$

Simple $\chi^2$ fitting is ill defined

Maximum Entropy Method

Regularize $\chi^2$ fitting by incorporating prior information

Check what parts of the spectrum depend on the regularization!
Extracting the Potential from Lattice QCD II

\[ \tau \in [0, \beta] \]

\[ x, y, z \]

\[ T < T_c \]

\[ V^{(0)}(R) \]

\[ \rho \]

\[ \omega \]

\[ T \approx T_c \]

\[ \text{Re}[V^{(0)}(R)] \]

\[ \text{Im}[V^{(0)}(R)] \]
First Numerical results

Quenched QCD Simulations
- Anisotropic Wilson Plaquette Action
- $T=0.78TC, 1.17TC, 2.33TC$
- $NX=20 \ \beta=6.1 \ \xi_b=3.2108 \ NT=36, 24, 12$
- Box Size: 2fm Lattice Spacing: 0.1fm
- HB:OR 1:4 with 200 sweeps/readout

Spectral Peak Fit
- Breit-Wigner and Gaussian shape
- Error bars from prior dependence

Maximum Entropy Method
- $N_\omega=1500, \ Prior: m_0/\omega, \ varied \ over \ 4 \ orders$
- Extended search space: decoupled from $N_T$
- Arbitrary precision arithmetic: 384bit
- Test I: Vary the prior amplitude
- Test II: Use different $N_T$
The Potential at $T=0.78T_C$

Prior dependence

MEM ringing
The Potential at $T=1.17T_C$

At $T>T_C$ upward trend

Only lowest peak stable

MEM ringing

Re$[V(R)]$ Im$[V(R)]$

$F^1(R)$
The Potential at $T=2.33T_C$

MEM stable but individual peaks overlapping

$\rho_\omega(\omega)$

$V_J(r) [\text{GeV}]$

$r [\text{fm}]$

$T=1.17T_C$

$\mathbf{Re}[V(R)]$ (\(\beta=7\))

$\mathbf{Im}[V(R)]$ (\(\beta=7\))

$\mathbf{Re}[V(R)]$

$\mathbf{Im}[V(R)]$
Static heavy quark potential derived from QCD

- Values can be extracted from Lattice QCD: Wilson loop spectral functions
- Spectral width / Imaginary part present above $T_C$
- Current numerical evaluation seems to favor strong imaginary part at $T>T_C$

Test extraction from spectral functions on HTL Wilson loop data/spectra

Include dynamical fermions for more realistic screening effects

work in progress with Y. Burnier
work in progress with O. Kaczmarek
A new proposal: width in the spectral function ↔ uncertainty in Re[V(R)]

At each time step the **purely real** potential V(R) is distorted by thermal fluctuations

Construct unitary stochastic time evolution (neglects back reaction on medium)

\[
\Psi_{\bar{Q}Q}(\mathbf{R}, t) = \mathcal{T} \exp \left[ -\frac{i}{\hbar} \int_0^t dt \left\{ -\frac{\nabla^2}{2m_Q} + V(\mathbf{R}) + \Theta(\mathbf{R}, t) \right\} \right] \Psi_{\bar{Q}Q}(\mathbf{R}, 0)
\]

\[
\langle \Theta(\mathbf{R}, t) \rangle = 0, \quad \langle \Theta(\mathbf{R}, t) \Theta(\mathbf{R}', t') \rangle = \hbar \Gamma(\mathbf{R}, \mathbf{R}') \delta_{tt'} / \Delta t
\]
Heavy Quarkonia as Open Quantum System

- Underlying theoretical framework: Open Quantum Systems
  - Change of notation: $\rho(t)$ density matrix of states
    $$H = H_{\text{sys}} \otimes I_{\text{med}} + I_{\text{sys}} \otimes H_{\text{med}} + H_{\text{int}}$$
    $$\frac{d}{dt} \rho(t) = \frac{1}{i\hbar} [H, \rho(t)]$$  unitary evolution: $H=H^\dagger$

- Interested in the dynamics of the QQbar system only
  $$\rho_{QQ}(t, \mathbf{R}, \mathbf{R}^\prime) = \text{Tr}_{\text{med}} \left[ \rho(t, \mathbf{R}, \mathbf{R}^\prime) \right]$$
  $$= \langle \Psi_{QQ}(\mathbf{R}, t) \Psi_{QQ}^* (\mathbf{R}^\prime, t) \rangle_{\Theta}$$

- Interaction with the medium induces a stochastic element into the dynamics
  (similar concepts are quantum state diffusion, quantum jumps, etc..)

- Decoherence: Interaction between medium and QQbar select a basis of states in which $\rho_{QQ}$ becomes diagonal over time

see e.g. H.-P. Breuer, F. Petruccione, Theory of Open Quantum Systems

see also: N.Borghini, C.Gombeaud: arXiv:1109.4271
Time evolution of Heavy Quarkonium

- Evolution on the level of the wavefunction:
  \[ i \frac{d}{dt} \Psi_{QQ}(R, t) = \left( -\frac{\nabla^2}{2\mu} + V(R) + \Theta(R, t) - i \frac{\Delta t}{2} \Theta^2(R, t) \right) \Psi_{QQ}(R, t) \]

- Average wavefunction only depends on diagonal correlations
  \[ i \frac{d}{dt} \langle \Psi_{QQ}(R, t) \rangle_\Theta = \left( -\frac{\nabla^2}{2\mu} + V(R) - i \frac{1}{2} \Gamma(R, R) \right) \langle \Psi_{QQ}(R, t) \rangle_\Theta \]

- Evolution on the level of the density matrix:
  - Averaged quantity whose time evolution depends on off-diagonal \( \Gamma(R, R') \)
  - How to extract information about \( \Gamma(R, R') \) from the lattice

- Survival probability of Heavy Quarkonia  
  (Vacuum: \( H^{\text{vac}} \)  QGP: \( H \))
  - Admixture \( c^\nu_{nm}(t) \) of initial bound eigenstates \( \Phi_n \) of \( H^{\text{vac}} \) at the current time

\[ c^\nu_{nm}(t) = \int dR dR' \ \Phi_n^*(R) \langle \Psi_{QQ}(R, t) \rangle_\Theta \Phi_n(R') \quad \rightarrow \quad P^\nu(t) = \sum_{n \text{ bound}} c^\nu_{nn}(t) \]
**First numerical 1-d calculations**

- QQbar in vacuum: Cornell potential with string breaking $\sigma=(0.4\text{GeV})^2 \ r_{sb}=1.5\text{fm}$
- Determine vacuum ground state
  - PETSC+SLEPC eigensystems

- Dynamics governed by different model potentials ($T=2.33T_C$):
  - All thermal effects in the noise, real part similar to vacuum
  - Debye screening and small noise ($m_D\approx1\text{GeV}$) *(Laine et. al. 2007)*
  - Pure Debye screening without noise ($m_D=5\text{GeV}$) *(Matsui, Satz, 1986)*

**Stochastic Dynamics**
- Crank-Nicholson algorithm in 1 dimension
- $N=512, \ dx=0.01\text{fm}, \ dt=dx/100\text{ fm}$
- Diagonal noise: too small correlation length
Generic features of the simulation

Unitarity is preserved in each member of the stochastic ensemble \( <|\Psi_{QQ}|> = 1 \)

Imaginary part emerges after averaging \( |<\Psi_{QQ}>| < 1 \)

Diagonal noise: Correlation length \( l_{corr} = dx << 2\pi/T \)
Heavy quarkonium in the QGP I

- Exponential suppression in $P^{v}(t)$: $v(x)$ and $\Gamma(x,x)$ determine speed
- Populating of higher states: Noise vs. mixing through $h(x)$
- Very different parameter sets give similar asymptotic $P^{v}(t) \rightarrow$ artificial
Heavy quarkonium in the QGP II

- Mixing through $h(x)$ with $m_D=5\text{GeV}$
- Observed suppression not exponential, not even monotonous
- Only parity even eigenstates are excited
Conclusion and Outlook

- Static heavy quark potential derived from QCD
  - Values can be extracted from Lattice QCD: Wilson loop spectral functions
  - Spectral width / Imaginary part present above $T_C$
  - Current numerical evaluation seems to favor strong imaginary part at $T>T_C$

  Test extraction from spectral functions on HTL Wilson loop data/spectra
  - work in progress with Y. Burnier

  Include dynamical fermions for more realistic screening effects
  - work in progress with O. Kaczmarek

- Stochastic evolution of Heavy Quarkonia in the QGP
  - Instead of imaginary part: uncertainty in the real part of the potential
  - Microscopic evolution fully unitary, $\text{Im}[V]$ obtained after ensemble average

  3d-simulation, LQCD determination of $\Gamma(R,R')$, incorporate drift term ...
Additional Slides
An alternative observable

- Derivation of $V(R)$ remains the same
- Lattice data much less noisy
- Real part and width are smaller
  - Possible tradeoff to ensure same physics outcome?
Extracting the Potential from Lattice QCD I

- We can measure neither $\rho_{\Box}(R,\omega)$ nor $W_{\Box}(R,t)$ directly in Lattice QCD

$$W_{\Box}(R,t) = \int_{-\infty}^{\infty} d\omega \ e^{-i\omega t} \rho_{\Box}(R,\omega)$$

- Simple $\chi^2$ fitting is ill defined

- Bayes Theorem (Maximum Entropy Method)

$$P[\rho|Dh] = \frac{P[D|\rho h] P[\rho|h]}{P[D|h]}$$

- Regularize $\chi^2$ fitting through entropy

$$\propto \exp \left[ -\frac{1}{2} \sum_{ij} \left( D(\tau_i) - D_\rho(\tau_i) \right) C_{ij}^{-1} \left( D(\tau_j) - D_\rho(\tau_j) \right) \right]$$

Likelihood: the usual $\chi^2$ fitting term

$$\frac{\delta}{\delta \rho} P[\rho|Dh] = 0$$

$$\propto \exp \left[ \int_{-\infty}^{\infty} \left\{ \rho(\omega) - h(\omega) - \rho(\omega) \log \left( \frac{\rho(\omega)}{h(\omega)} \right) \right\} d\omega \right]$$

Prior probability: Shannon-Janes entropy

Extended search space: decouple from $N_t$
Towards more realistic noise

- On the right: correlation length $l_{corr} = 4dx$, $\Gamma(x,x') \propto \exp[-|x-x'|^2/l_{corr}^2]$
- Noise less localized: ground state suppression slower
- Population of states follows eigenenergy scale ($t<10fm$)
Comparison: Stochastic $V(R)$ vs. $\text{Im}[V](R)$

- **Debye screening + small noise**
- **Debye screening with explicit $\text{Im}[V]$**

- **At early times:** similar evolution
- **At late times very distinct:** finite suppression vs. unabated decrease
- **Need to include backreaction physics to understand $P^v(t)$**