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From OQS to Quantum Trajectories for Quarkonia

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October 2023









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MAC.



Can we describe how quarkonia propagates through a medium from *first principles*?

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Can we describe how quarkonia propagates through a medium from *first principles*?

We can try! Open Quantum Systems can help us outline a method to do so.





They are **bound states of a heavy quark-antiquark pair** (QQ) **of the same kind** (Olsen et al., 2017) which are stable with respect to strong decay into open charm/bottom (Sarkar et al., 2010).



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Experimental evidence (Chatrchyan et al., 2012) of nuclear effects in the creation and propagation of quarkonia.



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Why choosing quarkonia as a probe?



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Why choosing quarkonia as a probe?

• Hard scale: quarkonia mass $m_{Q\bar{Q}}, m_Q \gg \Lambda_{QCD}$. Easy to be described by EFT.

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Why choosing quarkonia as a probe?

- Hard scale: quarkonia mass $m_{Q\bar{Q}}, m_Q \gg \Lambda_{QCD}$. Easy to be described by EFT.
- e Harder to dissociate from color screening than light quark matter.

$$\Delta E_{J/\psi} = 2M_D - M_{J/\psi} \approx 0.6 \text{ GeV} \gg \Lambda_{QCD} \approx 0.2 \text{ GeV}.$$
 (1)

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Well-known probe. Experimentally, clean signal through dilepton decays.

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<u>Open Quantum Systems 101</u>

We divide the full quantum system (T) into well-differentiated parts: the subsystem (S) and the environment (E) (Breuer and Petruccione, 2002).

The full quantum dynamics of the subsystem, a bound state, is kept whereas the environment is traced out.



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<u>Open Quantum Systems 101</u>

We divide the full quantum system (T) into well-differentiated parts: the subsystem (S) and the environment (E) (Breuer and Petruccione, 2002).

The full quantum dynamics of the subsystem, a bound state, is kept whereas the environment is traced out.



Main character (density matrix, ρ) and observables $\langle \mathcal{O} \rangle$:

$$\rho = p_i \sum_i |\psi_i\rangle \langle \psi_i| \longrightarrow \langle \mathcal{O} \rangle = Tr\{\rho \mathcal{O}\}.$$
 (2)

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Hamiltonian: $H_T = H_S \otimes \mathbb{I}_F + \mathbb{I}_S \otimes H_F + H_I$, where $H_I = V_S \otimes V_F$. ◆□▶ ◆□▶ ◆□▶ ◆□▶ → □ ・ つくぐ

The explicit form of the full hamiltonian (using LO NRQCD in the Coulomb gauge) would be:

$$H_{T} = \frac{1}{2M} \left(p_{Q}^{2} + p_{\bar{Q}}^{2} \right) \otimes \mathbb{I}_{E} + \mathbb{I}_{S} \otimes H_{q+A} + \int d^{3}x [\delta(\mathbf{x} - \mathbf{x}_{Q})t_{Q}^{a} - \delta(\mathbf{x} - \mathbf{x}_{\bar{Q}})t_{Q}^{a*}] \otimes gA_{0}^{a}(\mathbf{x})$$
(3)

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(3)

We know that:

$$Tr_E\Big[T[A_0^a(t_1,\mathbf{x}_1)A_0^b(t_2,\mathbf{x}_2)]\rho_E\Big] = -i\delta^{ab}\Delta(t_1-t_2,\mathbf{x}_1-\mathbf{x}_2) \quad (4)$$

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We know that:

$$Tr_E\Big[T[A_0^a(t_1,\mathbf{x}_1)A_0^b(t_2,\mathbf{x}_2)]\rho_E\Big] = -i\delta^{ab}\Delta(t_1-t_2,\mathbf{x}_1-\mathbf{x}_2) \quad (4)$$

We can profit from the fact that propagators of the A_0 component can be linked with real and imaginary potentials like (Blaizot and Escobedo, 2017):

$$V(\mathbf{r}) = -\Delta^{R}(\omega = 0, \mathbf{r}), \qquad W(\mathbf{r}) = -\Delta^{<}(\omega = 0, \mathbf{r}) \tag{5}$$

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$$\frac{d}{dt}\rho_{T}(t) = -i[H_{T}, \rho_{T}(t)] \Longrightarrow \rho_{T}(t) = -i\int_{0}^{\infty} dt'[H_{T}, \rho_{T}] \quad (6)$$

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Go to the interaction picture.

$$\frac{d}{dt}\rho_{T}(t) = -i[H_{T}, \rho_{T}(t)] \Longrightarrow \rho_{T}(t) = -i\int_{0}^{\infty} dt'[H_{T}, \rho_{T}] \quad (6)$$

Go to the interaction picture.

Iterate the integral equation into the differential one.

$$\frac{d\rho_{I,T}(t)}{dt} = -\int_0^t dt' [H_I(t), [H_I(t'), \rho_{I,T}(t')]]$$
(7)

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Oivide DoF into subsystem + environment.

Evolution: Liouville - von Neumann equation.

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Iterate the integral equation into the differential one.

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(7)

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- Oivide DoF into subsystem + environment.
- Trace out the environmental DoF \longrightarrow loss of unitarity. $Tr_E[\rho_T] = \rho_S$



Further approximations can be done which also refer to the characteristic timescales τ_i of the system, namely:

$$au_{S} = 1/\Delta E, \quad au_{E} \sim 1/T, \quad au_{R} \sim M/T^{2}.$$
 (9)

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Here ΔE is the energy gap between the energy levels of the bound state, T is the temperature and M is the particle mass.



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$$au_E \ll au_R \longrightarrow$$
 Born and Markov approximations. (10)

$$\tau_E \ll \tau_S \longrightarrow \text{Born-Oppenheimer approximation.}$$
 (11)

These considerations will help out with the algebraic manipulations to reach the desired and consistent OQS shape of the equation of evolution.

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$$\left|\frac{d\rho_{\mathcal{S}}(t)}{dt}=-\int_{0}^{t}dt' \operatorname{Tr}_{\mathcal{E}}\left[\left[H_{l}(t),\left[H_{l}(t'),\rho_{l,T}(t')\right]\right]\right]\right|$$

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$$\frac{d\rho_{\mathsf{S}}(t)}{dt} = -\int_0^t dt' \operatorname{Tr}_{\mathsf{E}}\left[\left[H_l(t), \left[H_l(t'), \rho_{l,\mathsf{T}}(t')\right]\right]\right]$$

$$\rho_{T}(t) \approx \rho_{S}(t) \otimes \rho_{E}(t) \approx \rho_{S}(t) \otimes \rho_{E}(0)$$
(13)

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2 Markov approximation \longrightarrow no memory in the system.

$$(0,t) \longrightarrow (-\infty,0), \quad \rho_T(t') \approx \rho_T(t)$$
 (14)

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$$\frac{d\rho_{\mathcal{S}}(t)}{dt} = -\int_0^t dt' \operatorname{Tr}_{\mathcal{E}}\left[\left[H_l(t), \left[H_l(t'), \rho_{l,T}(t')\right]\right]\right]$$

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(13)

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 (14)

Sorn-Oppenheimer approximation → the light degrees of freedom of the plasma accommodate very fast to changes produced by quarkonia (~ atomic physics).

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As a result, after some rearranging, we get the Lindblad equation:

$$\frac{d\rho_{\mathcal{S}}(t)}{dt} = -i[H_{\mathcal{S}}(t),\rho_{\mathcal{S}}(t)] + \sum_{k} \left(L_{k}\rho_{\mathcal{S}}L_{k}^{\dagger} - \frac{1}{2} \{ L_{k}^{\dagger}L_{k},\rho_{\mathcal{S}}(t) \} \right), \quad (15)$$

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As a result, after some rearranging, we get the Lindblad equation:

$$\frac{d\rho_{\mathcal{S}}(t)}{dt} = -i[H_{\mathcal{S}}(t),\rho_{\mathcal{S}}(t)] + \sum_{k} \left(L_{k}\rho_{\mathcal{S}}L_{k}^{\dagger} - \frac{1}{2} \{ L_{k}^{\dagger}L_{k},\rho_{\mathcal{S}}(t) \} \right), \quad (15)$$

 $L_k \sim D_{env.}(t, \mathbf{x}) \cdot (V_S^k(t) + \frac{i}{4T} \frac{dV_S^k(t)}{dt})$ is called the Lindblad operator (Akamatsu, 2022).

- **(**) k > 1, if more than one kind of operator (decay channel).
- 2 $D_{env.}(t, \mathbf{x}) \sim \Delta(t, \mathbf{x})$, from tracing out the environmental DoF.

Conceptually, Lindblad operators are going to produce **jumps** between states (modifying the internal quantum numbers of the system). Thus, they are also called **jump operators**.



We redefine the subsystem hamiltonian by adding the 1-loop contributions, H_{1-loop} (Akamatsu, 2022; Blaizot and Escobedo, 2018; Yao and Mehen, 2019).

It becomes a non-hermitian hamiltonian.

$$H_{eff} = H_S + H_{1-loop} = H_S - \frac{l}{2} \sum_k \gamma_k \mathcal{L}_k^{\dagger} \mathcal{L}_k$$
(16)

$$\frac{d\rho_{S}(t)}{dt} = -i[H_{eff}(t), \rho_{S}(t)] + \sum_{k} L_{k} \rho_{S} L_{k}^{\dagger}, \qquad (17)$$

The state is evolved in Schrödinger-like way (norm decreases). When the norm goes below a certain value, a projection (jump) is performed according to certain selection rules.



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Description of the algorithm



 Non-hermitian hamiltonian evolution step is performed. Its non-unitarity makes the norm of the state decrease.

 $\langle \psi(t_1) | \psi(t_1) \rangle > \langle \psi(t_2) | \psi(t_2) \rangle$, where $t_1 < t_2$ (18)

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 $\langle \psi(t_1) | \psi(t_1) \rangle > \langle \psi(t_2) | \psi(t_2) \rangle$, where $t_1 < t_2$ (18)

A random number decides if the jump is performed. The state will normally evolve until the norm goes below this value.

When $\langle \psi(t) | \psi(t) \rangle < \text{Random Number} \longrightarrow \text{jump.}$ (19)

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When $\langle \psi(t) | \psi(t) \rangle < \text{Random Number} \longrightarrow \text{jump.}$ (19)

Randomly select the jump according to certain selection rules.
 We project using the corresponding jump operator:

$$|\psi_{new}\rangle = \hat{L}^{x}(\vec{q}) |\psi_{old}\rangle$$
(20)

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Context Open Quantum Systems Quantum Trajectories New Implementation Wrap-up and References Appendix 000000 Description of the algorithm

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$$|\psi_{new}\rangle = \hat{L}^{\times}(\vec{q}) |\psi_{old}\rangle$$
 (20)

Renormalize and back again.



Selection rules are enacted via the partial decay rates $\Gamma(p)$ (Blaizot and Escobedo, 2018). These explicitly depend on the shape of the Lindblad operators.



Decay rates are defined as:

$$\Gamma_k(p) = L_k(p)L_k^{\dagger}(p). \quad (21)$$

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QTRAJ 1.0 (Ba Omar et al., 2022): C-based code which simulates through the quantum trajectories algorithm and shows the relative population of colour and wave states for quarkonia.

The current potential available compatible with the Lindblad formalism is the Munich potential. This approach is adequate for a regime where $rT \ll 1$ and is performed with a finite number of Lindblad operators.

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The current potential available compatible with the Lindblad formalism is the Munich potential. This approach is adequate for a regime where $rT \ll 1$ and is performed with a finite number of Lindblad operators.

Goal of $+\epsilon$: New potentials \longrightarrow Infinite number of Lindblad operators \longrightarrow reach regime where $rT \approx 1$. **How?:**

- Adding definitions of new potentials to QTRAJ.
- ❷ Modifying the selection rules ↔ Defining new Lindblad operators.

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New potential, less restrictive, to try to perform up to $rT \approx 1$. We will use the general expression:

$$\Delta(\omega = 0, \mathbf{r}) = -\Delta^{R}(\omega = 0, \mathbf{r}) + i\Delta^{<}(\omega = 0, \mathbf{r}), \qquad (22)$$

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which was found when tracing out the environment to get the Lindblad operators.

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which was found when tracing out the environment to get the Lindblad operators. These correspond to real and imaginary potentials, in our case: .

$$Re\{H_I(r)\} = -C_F \alpha_s(1/a_0) \frac{e^{-m_D r}}{r}, \qquad (23)$$

$$Im\{H_{I}(r)\} = \frac{g^{2}T}{2\pi} \int_{0}^{\infty} dx \frac{x}{(x^{2}+1)^{2}} \Big[1 - \frac{\sin(xrm_{D})}{xrm_{D}} \Big]$$
(24)

where m_D is the Debye mass:

$$m_D = \sqrt{\frac{2N_c + N_f}{6}}gT \tag{25}$$

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Lindblad operators are in this framework:

$$\hat{L}^{x}(\vec{q}) = K_{x}\sqrt{\Delta(\vec{q})}cs(rac{\vec{q}\cdot\hat{\vec{r}}}{2}),$$
 (26)

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where cs stands for $\sin\left(\vec{q} \cdot \hat{\vec{r}}/2\right)$ if $x \in \{s \to o, o \to s, o \to o \ (1)\}$ and $\cos\left(\frac{\vec{q} \cdot \hat{\vec{r}}}{2}\right)$ is $x \in \{o \to o \ (2)\}$.

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$$\hat{L}^{\times}(\vec{q}) = K_{\times} \sqrt{\Delta(\vec{q})} cs(\frac{\vec{q} \cdot \hat{\vec{r}}}{2}), \qquad (26)$$

where cs stands for $\sin\left(\vec{q} \cdot \hat{\vec{r}}/2\right)$ if $x \in \{s \to o, o \to s, o \to o \ (1)\}$ and $\cos\left(\frac{\vec{q} \cdot \hat{\vec{r}}}{2}\right)$ is $x \in \{o \to o \ (2)\}$. Using:

$$e^{-i\vec{k}\vec{r}} = \sum_{\ell=0}^{\infty} (-i)^{\ell} j_{\ell}(kr) Y_{\ell m}(\vec{k}_{u}) Y_{\ell,m}^{*}(\vec{r}_{u}), \qquad (27)$$

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we get:

$$\hat{L}^{\times}(\vec{q}) = K_{\times} \sqrt{\Delta(\vec{q})} \sum_{t}^{\infty} \sum_{m=-\ell}^{\ell} j_{\ell}(qr) Y_{\ell}^{m}(\Omega_{r}) = \sum_{t}^{\infty} \hat{L}_{\alpha}^{\times}(\vec{q}), \quad (28)$$

where for the case of the cosine $\alpha = 2t$ and for the sine $\alpha = 2t + 1$.

New rules	

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The change affects how selection rules are implemented:



• We choose the kind of transition that quarkonia will undergo: apply the proper Lindblad operator:

$$\hat{L}^{s \longrightarrow o}(\vec{q}), \quad \hat{L}^{o \longrightarrow s}(\vec{q}), \quad , \hat{L}^{o \longrightarrow o(1)}(\vec{q}), \quad \hat{L}^{o \longrightarrow o(2)}(\vec{q}).$$
(29)

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② We choose the value of t of $\hat{L}_t^{\times}(\vec{q})$: virtual angular momentum of the one gluon exchange.



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$$\hat{L}^{s \longrightarrow o}(\vec{q}), \quad \hat{L}^{o \longrightarrow s}(\vec{q}), \quad , \hat{L}^{o \longrightarrow o(1)}(\vec{q}), \quad \hat{L}^{o \longrightarrow o(2)}(\vec{q}).$$
(29)

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- **②** We choose the value of t of $\hat{L}_t^{\times}(\vec{q})$: virtual angular momentum of the one gluon exchange.
- We choose *q* from its momentum distribution.



We choose the kind of transition that quarkonia will undergo: apply the proper Lindblad operator:

$$\hat{L}^{s \longrightarrow o}(\vec{q}), \quad \hat{L}^{o \longrightarrow s}(\vec{q}), \quad , \hat{L}^{o \longrightarrow o(1)}(\vec{q}), \quad \hat{L}^{o \longrightarrow o(2)}(\vec{q}).$$
(29)

- **②** We choose the value of t of $\hat{L}_t^{\times}(\vec{q})$: virtual angular momentum of the one gluon exchange.
- We choose *q* from its momentum distribution.
- We apply the Lindblad operator so:

$$\hat{L}_{t}^{x}(\vec{q}) |\psi_{old}\rangle = |\psi_{new}\rangle.$$
(30)

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Behaviour of the jump operators



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 Tendency of the jumps
 Jump



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Appendix

Plots that can be retrieved.



These results are from Strickland's original code (Brambilla et al., 2022).



- The inclusion of less restrictive potentials allows the expansion the regime of validity of the simulations.
- This means two things: either temperature does not have to be as high as before for applying this formalism or the small dipole approximation implicit in the Boltzmann equation is no longer applied. The latter case is of our greater interest.

The new shape of the Lindblad operators depend on the momentum exchanged with the medium particles. In the region of interest, ΔJ = 1 dominates.

Thank you!

New Implementation

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Appendix ●00000



It is a weak coupling between the subsystem and the environment, $H_{l} \ll 1$.

$$\rho_{T}(t) = \rho_{S}(t) \otimes \rho_{E}(t) + \rho_{corr}(t) \approx \rho_{S}(t) \otimes \rho_{E}(t), \qquad (31)$$

where $\rho_{\it corr}$ is the correlation component between the environment and the subsystem.

$$\frac{d\rho_{T,I}(t)}{dt} \approx -\int_0^t d\tau [H_I(t), [H_I(\tau), \rho_{S,I}(\tau) \otimes \rho_{E,I}(0)]]$$
(32)

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Approximations: Markov approximation

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Taking into account only the current step in order to obtain the next one $\rho_{S,I}(\tau) \longrightarrow \rho_{S,I}(t)$. We will perform the change of variable $\tau \longrightarrow \tau' = t - \tau$ so:

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$$\tau = 0 \longrightarrow \tau' = t - \tau = t$$

•
$$\tau = t \longrightarrow \tau' = t - \tau = 0$$

• Since the correlation time of the environment is much less than the average relaxation time of the system we can take $t \longrightarrow \infty$.

If we also trace over the environment, we get:

$$\frac{d\rho_{S,I}(t)}{dt} \approx -\int_0^\infty d\tau \ tr_E\{[H_I(t), [H_I(t-\tau), \rho_{S,I}(t) \otimes \rho_{E,I}(0)]]\}.$$
(33)

Redfield equation.

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The environmental degrees of freedom move much faster than the quarkonium so effectively they instantly change to any changes that the quarkonium may induce.

$$V_{\mathcal{S}}(t-s) \approx V_{\mathcal{S}}(t) - s \frac{dV_{\mathcal{S}}(t)}{dt} + \cdots = V_{\mathcal{S}}(t) - is[H_{\mathcal{S}}, V_{\mathcal{S}}(t)] + \dots$$
(34)

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Gradient expansion for Brownian motion.

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- **1** Projecting $\rho_{S}(t)$ into spherical harmonics.
- Also, split into the singlet-octet colour basis.

$$\rho_{\mathcal{S}}(t) = diag(\rho_{\mathcal{S}}^{sing,s}, \rho_{\mathcal{S}}^{oct,s}, \rho_{\mathcal{S}}^{sing,p}, \rho_{\mathcal{S}}^{oct,p})$$
(35)

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Great computational advantage: $3D \longrightarrow 1D \cdot Y_m^{\ell}(\theta, \phi)$.

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It is a deconfined phase on the QCD phase diagram [12].



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