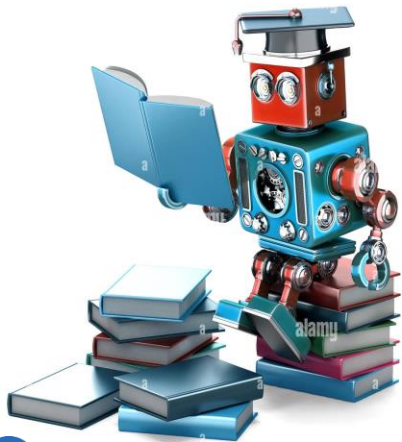


## Transport properties of the QGP matter facilitated by Machine learning-based models



Olga Soloveva, Andrea Palermo,  
Elena Bratkovskaya

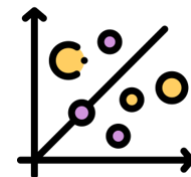
29 September, 2023  
2nd Workshop of the Network  
NA7-HF-QGP  
HFHF Theory Retreat 2023



# Main objectives for a ML framework in theory



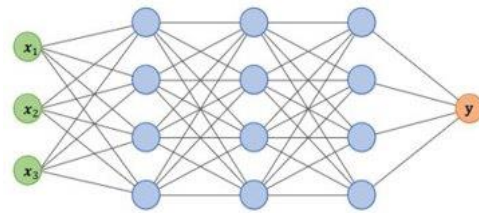
- Consistent framework (based on popular TensorFlow) for (on) off-shell model - simultaneously evaluate the EoS and transport coefficients of QGP to reduce model assumptions
- Create a faster framework to tune quasi-particle particle model parameters – can be easily **adjusted for other models**
- Check how strangeness is described within the quasi-particle models and its influence on transport coefficients
- Where can we gain knowledge from ML techniques (Unsupervised learning) for QGP phenomenology by the use of **regression task** not only classification?



# Unsupervised learning to explore the QGP

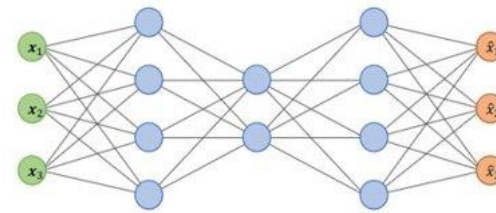
Popular types of NN used for phenomenology:

Regression/classification:



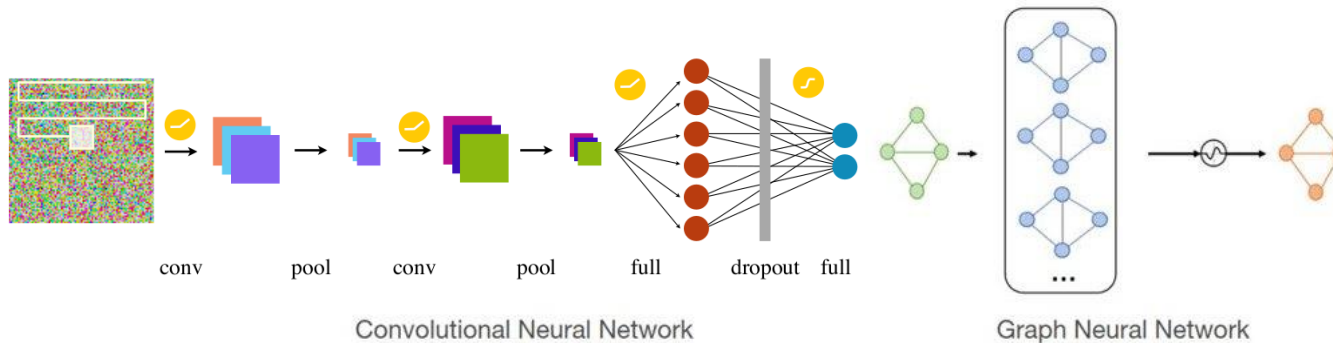
Deep Neural Network

Classification:



AutoEncoder

Fast simulations:  
CNN, new - GAN

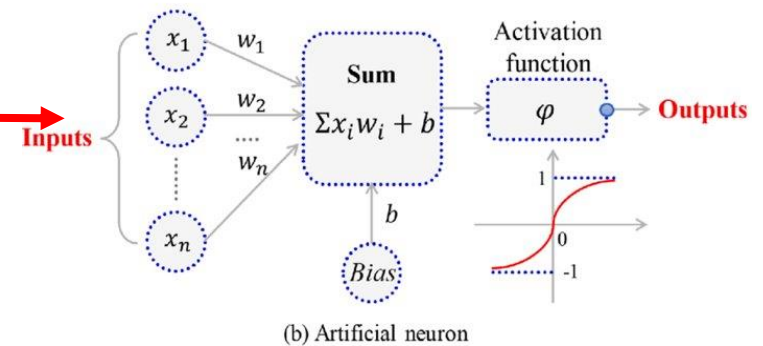
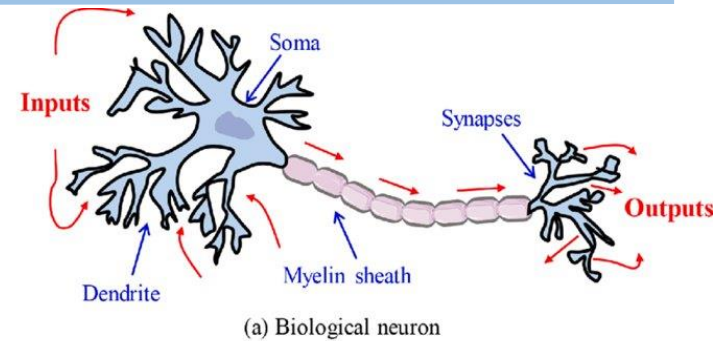
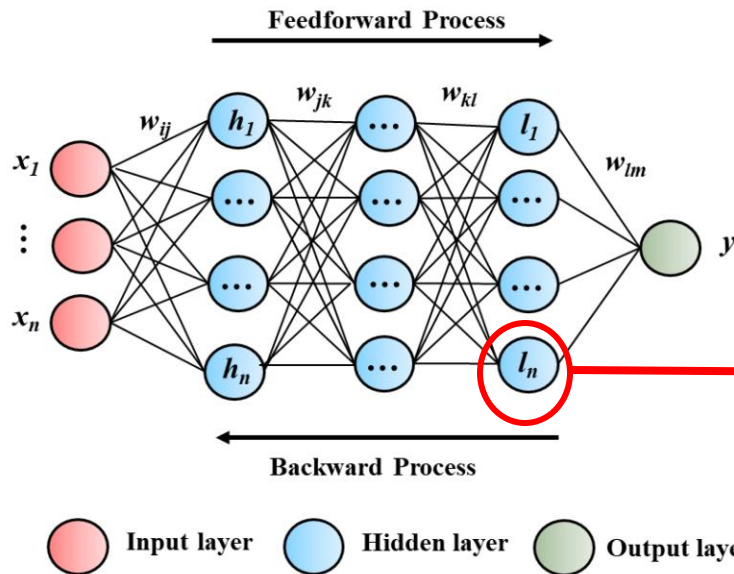


Convolutional Neural Network

Graph Neural Network

- Unsupervised Learning is most promising/suitable for phenomenology / theory of nuclear physics
- Can we use Unsupervised Learning to learn about the **dynamical properties of the QGP?**
- Exploring QCD matter in extreme conditions with Machine Learning (recent review: <https://arxiv.org/abs/2303.15136>)

# Machine Learning: Basic concepts



- **Forward propagation:** Transmission of input data resulting in an unsettled verdict
- **Loss estimation:** loss/cost function = discrepancy between predicted and actual values
- **Back propagation:** weights are iteratively refined to reduce the error
- **Optimization:** gradient descent (Adam) for correcting the weights

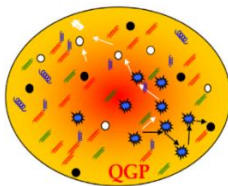
$$w \leftarrow w - \eta \frac{\partial l}{\partial w}$$

Objection: to minimize the loss of prediction on new data not used for trainings - we want to have some smooth loss function for optimization

- NN is a new tool for multidimensional optimization function which are more flexible and can encompass more features itself, and can be constructed in a more flexible manner than conventional optimization techniques

# Can ML be useful for theory of the QGP?

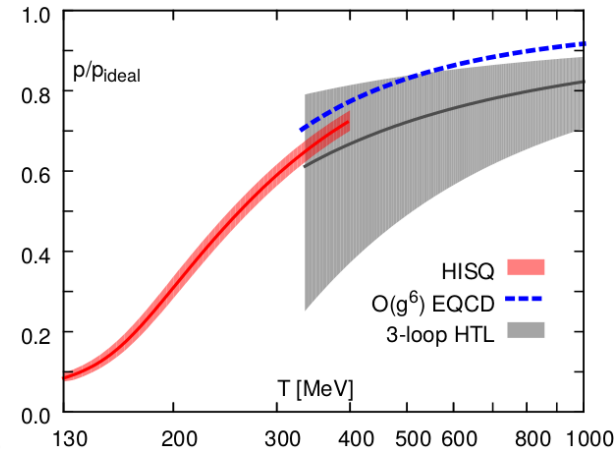
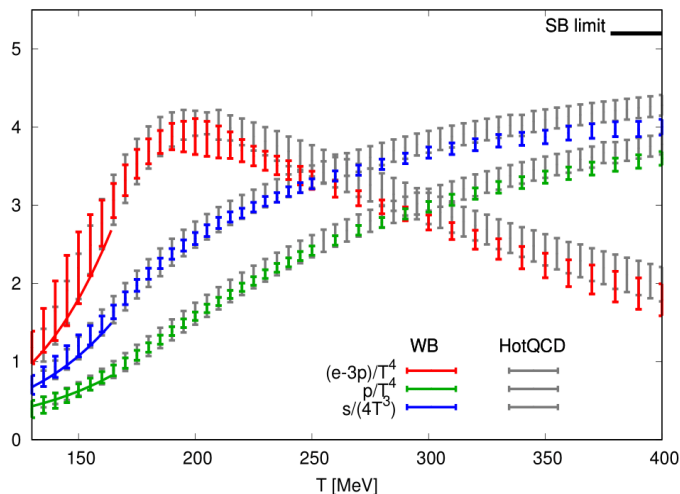
On practice: effective models  
for QGP



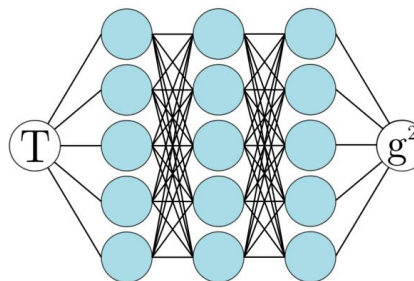
$$\begin{aligned} & \text{EoS}(\epsilon, n) \\ & \sigma(\sqrt{s}, m_q, m_q, T, \mu_B) \\ & m(T, \mu_B) \end{aligned}$$

**!** QPM enables to estimate simultaneously of the EoS and transport coefficients also including jet and charm coefficients (talk by **I Grishmanovskii**)

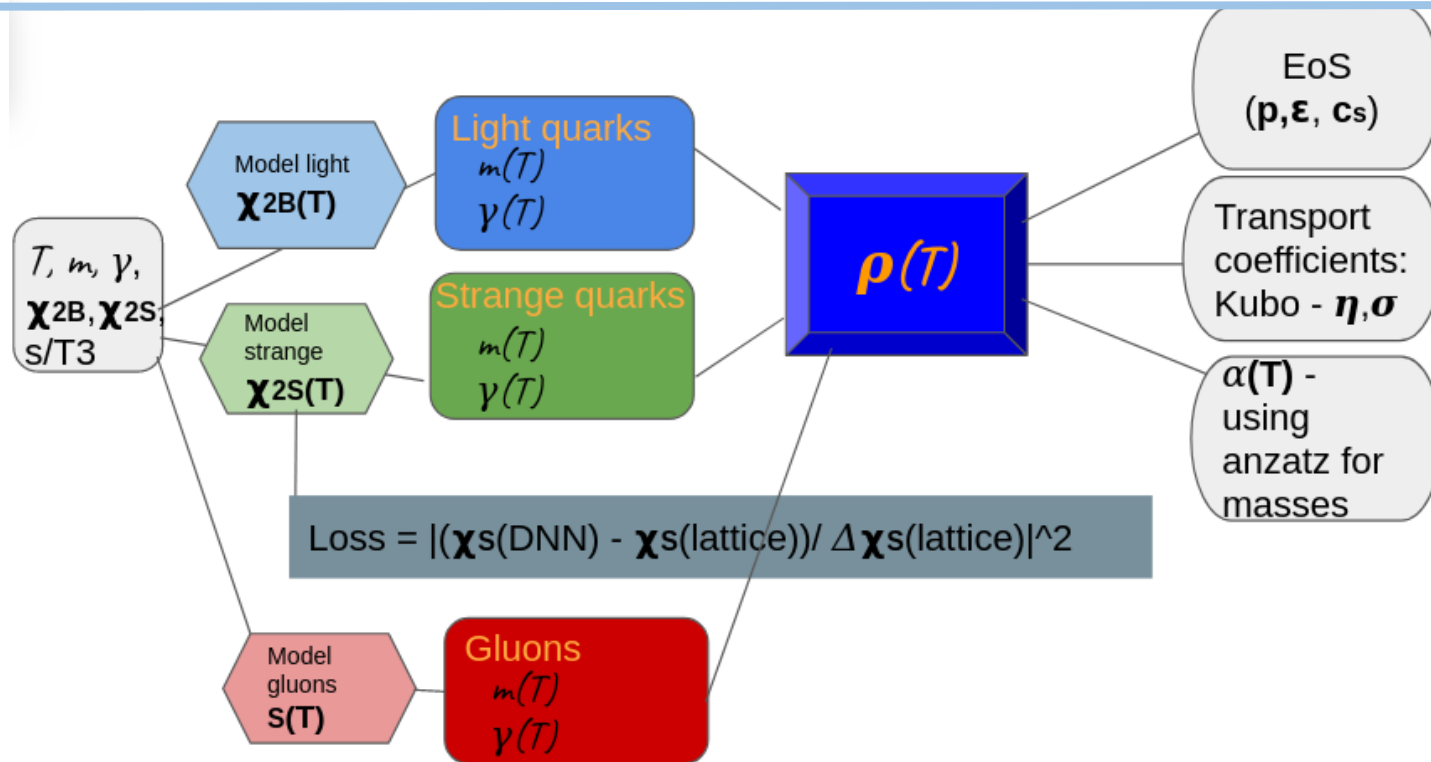
Phenomenological models are based on lattice QCD thermodynamics



**ML facilitated** QGP description – by minimizing the loss function (can be chosen in various forms)  
Output: spectral function, coupling constant – which later can be used for the extraction of transport coefficients



# Regression task



For training we use:  $T$ , EoS(from IQCD as true value):  $s/T^3(T)$ ,  $\chi_2^B(T)$ ,  $\chi_2^S(T)$

**Goal:** Extract microscopic quantities using thermodynamic quantities from 1st principle calculation (here IQCD)

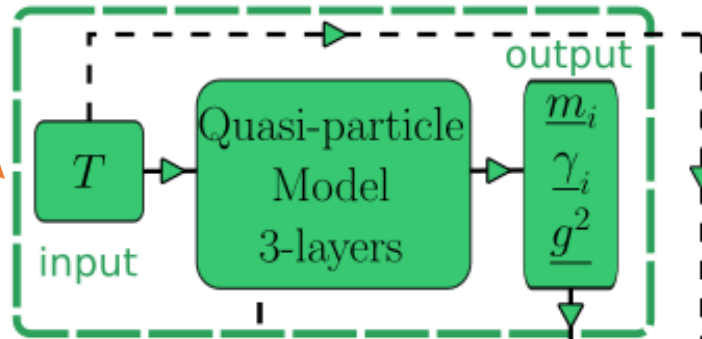
**Output:** masses, widths, coupling constant – which later can be used for the tuning quasiparticle models used for QGP phase in transport simulations and extraction of transport coefficients of the QGP phase

# Flowchart of DNN model

To train the DNN we generate tables with masses, widths and EoS using Off-shell quasi-particle description w/o any assumptions on masses and width

$T$	$\frac{M}{T} \in [\frac{\gamma}{T}, 9]$	$\frac{\gamma}{T} \in [0, 1]$	$I_B [GeV^3]$	$I_F [GeV^3]$	$\chi_q$
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Main DNN



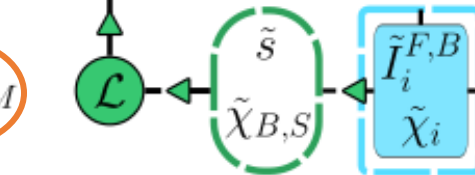
- Loss function to minimize

$$\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_{DQPM}$$

To improve physical meaning of the output:

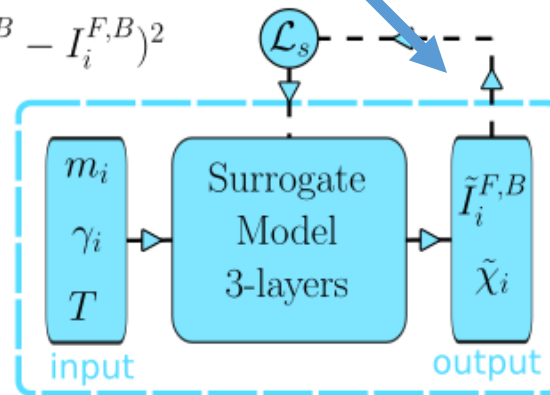
- Loss function can contain several terms:  $(\mathbf{y} - \mathbf{y}_{\text{true}})$  with  $[\mathbf{y}_{\text{true}} = \text{EoS}(\text{lattice})]$  and regularization terms

$[\mathbf{y}_{\text{true}} = \text{masses/widths (HTL) at high } T]$



2 Surrogate DNN

$$\mathcal{L}_s = \sum_i (I_i^{F,B} - \tilde{I}_i^{F,B})^2 + (\tilde{\chi}_i - \chi_i)^2$$



# Framework: off-shell Quasi-Particle Model

EoS from  $\Phi$  - functional approach - entropy and quark density and susceptibilities expressed in dressed propagators in the quasiparticle limit (G. Baym 1998, Blaizot et al. 2001):

$$s^{dqp} = - \int \frac{d\omega}{2\pi} \frac{d^3p}{(2\pi)^3} \left[ d_g \frac{\partial n_B}{\partial T} (\text{Im}(\ln \underline{-\Delta^{-1}}) + \text{Im} \underline{\Pi} \text{Re} \underline{\Delta}) + \sum_{q=u,d,s} d_q \frac{\partial n_F(\omega - \mu_q)}{\partial T} (\text{Im}(\ln \underline{-S_q^{-1}}) + \text{Im} \underline{\Sigma}_q \text{Re} \underline{S}_q) + \sum_{\bar{q}=\bar{u},\bar{d},\bar{s}} d_{\bar{q}} \frac{\partial n_F(\omega + \mu_q)}{\partial T} (\text{Im}(\ln \underline{-S_{\bar{q}}^{-1}}) + \text{Im} \underline{\Sigma}_{\bar{q}} \text{Re} \underline{S}_{\bar{q}}) \right]$$

- We need to estimate during training to estimate Loss

$$s(T) = -d_g I_g^B - d_q \sum_{i=q,s} I_i^F$$

$$\chi_2^B(T) = \frac{d_q}{9} (2\chi_l(T) + \chi_s),$$

$$\chi_2^S(T) = d_q \chi_s,$$

original DQPM model - QGP in the PHSD (Elena's talk) - coupling constant is fixed using entropy density

- Input: entropy density as a  $f(T, \mu_B = 0)$

$$g^2(s/s_{SB}) = d((s/s_{SB})^e - 1)^f$$

$$s^{DQPM}(\Pi, \Delta, S_q, \Sigma) = s^{lattice} \quad \text{fit S from QP to S from IQCD}$$

fix the model parameters

$$g^2(T/T_c, \mu_B) = g^2\left(\frac{T^*}{T_c(\mu_B)}, \mu_B = 0\right) \quad \text{with} \quad T^* = \sqrt{T^2 + \mu_q^2/\pi^2}$$

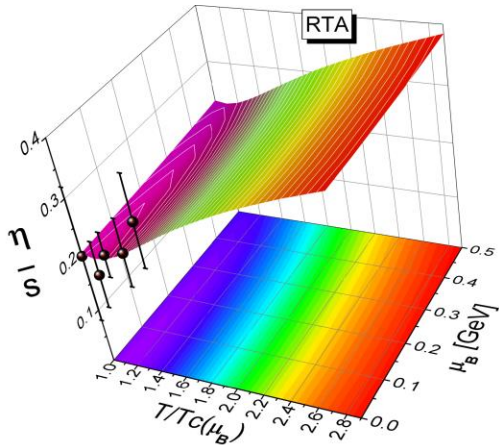
- Scaling hypothesis for the crossover region at finite  $\mu_B$



# DQPM: EoS and transport coefficientst

- DQPM: off-shell Quasi-Particle Model - can provide **simultaniously** **Transport coefficients + EoS**

O. S., P. Moreau and E. Bratkovskaya,  
PRC 101 (2020), 045203

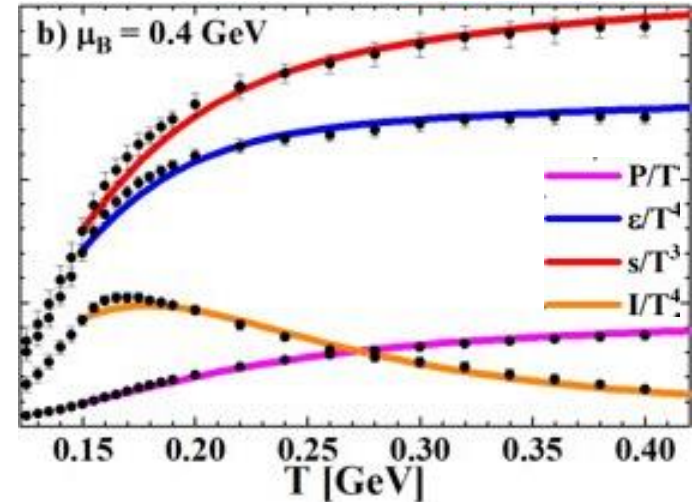


$$\eta \nabla^{\langle \mu} u^{\nu \rangle}$$

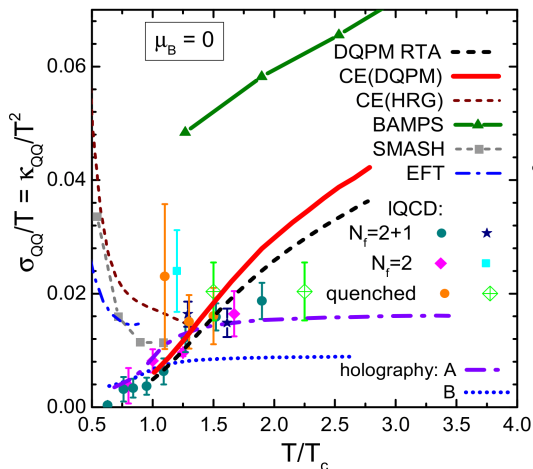
$$-\zeta \nabla u$$

(B, Q, S) diffusion coefficients

$$\kappa_q \nabla \frac{\mu_q}{T}$$



+ Full diffusion coefficient matrix



- Main thermodynamic quantities are within the errorbars in agreement with IQCD EoS at moderate
- Baryon and strange susceptibilities are lower than LQCD data- **improve!**
- **Improve strange quark description**

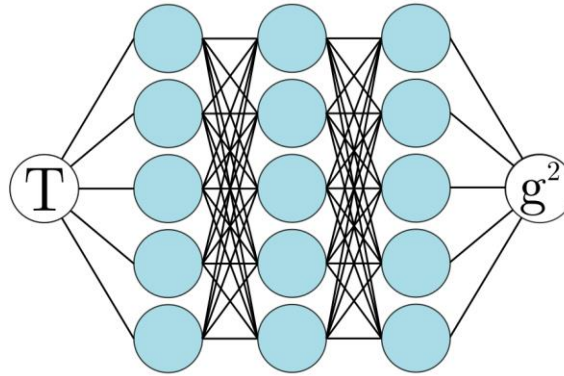
J. A. Fotakis, O. S., C. Greiner, O. Kaczmarek and E. Bratkovskaya PRD 104 (2021) , 034014

Cassing, NPA 791 (2007) 365; H. Berrehrah, E. Bratkovskaya, T. Steinert, W. Cassing, Int. J. Mod. Phys. E 25 (2016), 164200; P. Moreau, O. S., L. Oliva, T. Song, W. Cassing, E. Bratkovskaya, PRC 100 (2019) , 014911;

# DNN with Dynamical Quasi-Particle Model

## NN:

3 layers, 24x12x12x1 and swish/sigmoid



**Output:** coupling constant  
masses and widths falls from the DQPM Ansatz – in HTL form

Re  $\Pi_i$ : thermal mass ( $M_g, M_q$ )

$$m_g^2(T) = C_a \frac{g^2(T)}{6} T^2 \left( 1 + \frac{N_f}{2N_c} \right) = \frac{3}{4} g^2(T) T^2$$

$$m_{l(\bar{l})}^2(T) = C_f \frac{g^2(T)}{4} T^2 = \frac{1}{3} g^2(T) T^2$$

**Strange quark:**

$$m_{s(\bar{s})}(T) = m_{q(\bar{q})}(T) + \Delta m$$

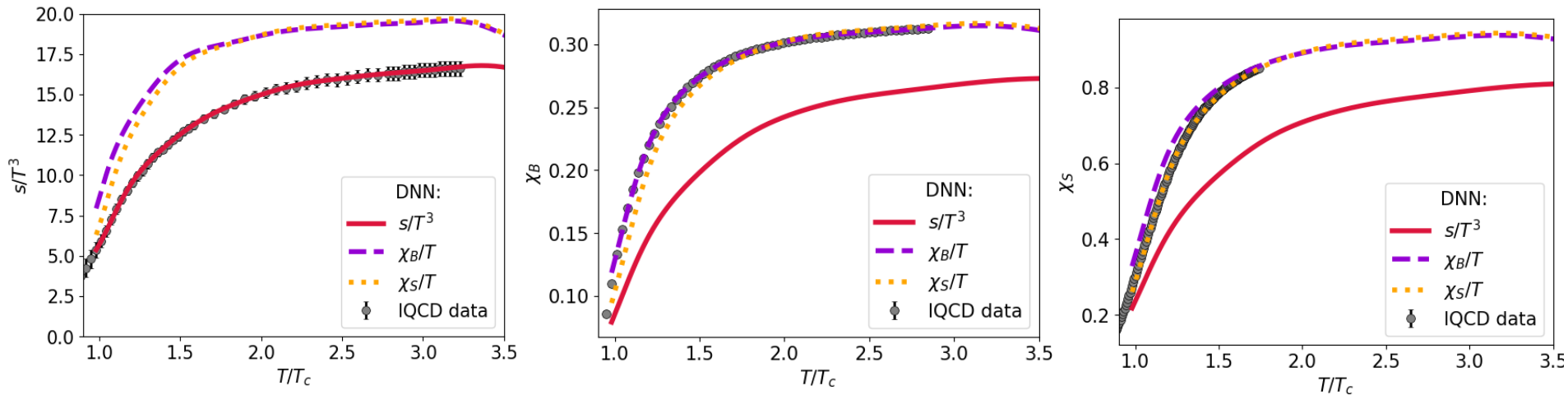
Im  $\Pi_i$  : interaction width ( $\gamma_g, \gamma_q$ )

$$\gamma_j(T, \mu_B) = \frac{1}{3} C_j \frac{g^2(T, \mu_B) T}{8\pi} \ln \left( \frac{2c_m}{g^2(T, \mu_B)} + 1 \right)$$

# EoS from DNN with DQPM Ansatz

- Loss function to minimize

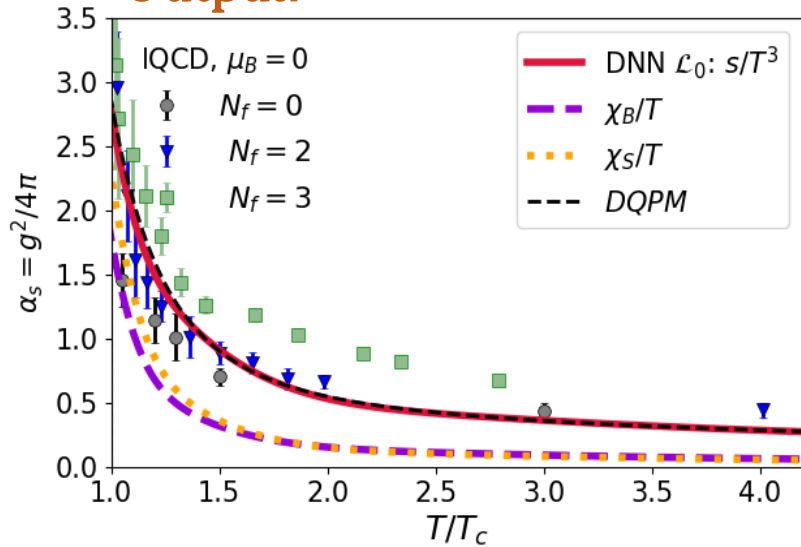
$$\mathcal{L}_0 = \beta_G \left[ \frac{\tilde{s}(T) - s_{\text{IQCD}}}{\Delta s_{\text{IQCD}}} \right]^2 + \beta_L \left[ \frac{\tilde{\chi}^B(T) - \chi_{\text{IQCD}}^B}{\Delta \chi_{\text{IQCD}}^B} \right]^2 + \beta_S \left[ \frac{\tilde{\chi}^S(T) - \chi_{\text{IQCD}}^S}{\Delta \chi_{\text{IQCD}}^S} \right]^2$$



- Impossible to fit all 3 and get not huge masses
- Simple consideration of different contribution – results in different estimations of effective coupling constant
- DNN: in which direction we can improve the model?

# Proof of principle: DQPM Ansatz

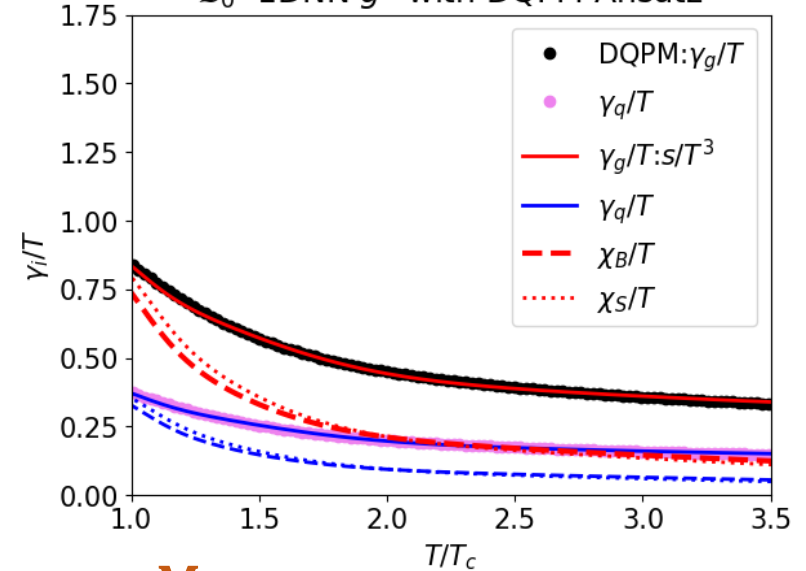
## Output:



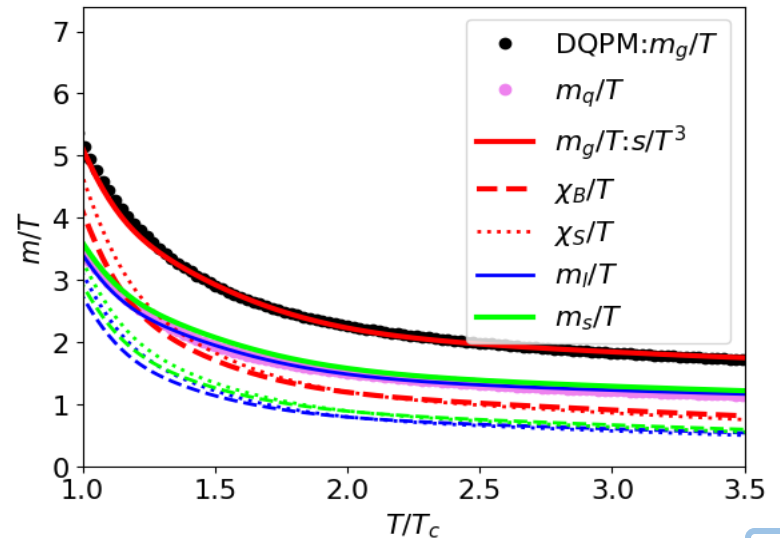
Possible improvements -

- change the form of Ansatz in that way to keep **masses/widths** in a **physical range**.
- change **width/mass** for strange quark

## $\mathcal{L}_0$ 1DNN $g^2$ with DQPM Ansatz



## Masses



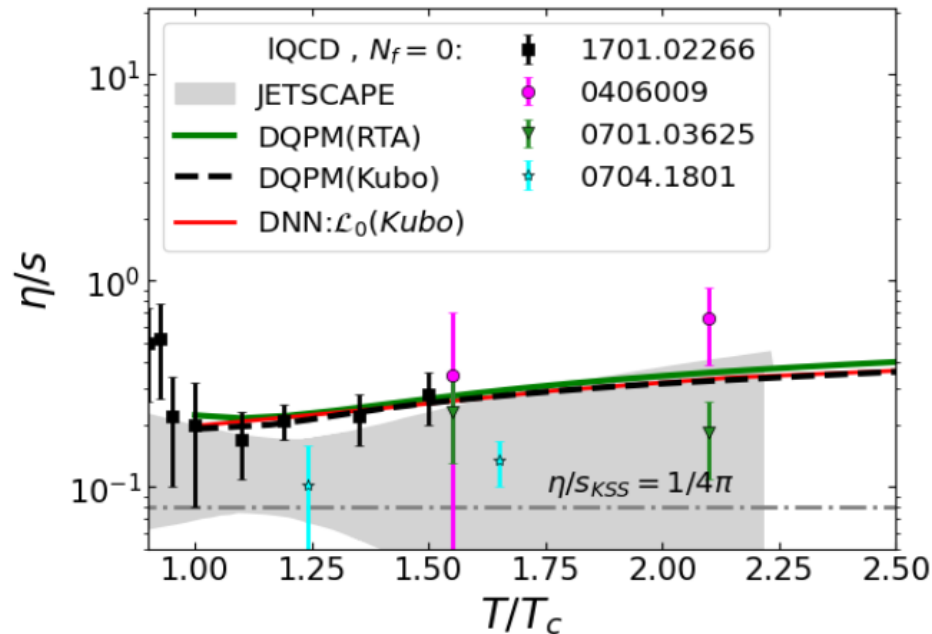
# Transport coefficients : Kubo formalism

$$\eta^{\text{Kubo}}(T) = \frac{1}{15T} \int \frac{d^4p}{(2\pi)^4} \sum_{i=q,\bar{q},g} d_i ((1 \pm f_i(\omega)) f_i(\omega)) \rho_i(\omega, \mathbf{p})^2 \Pi_i$$

Contain all degrees of freedom

$$\Pi_g = 7\omega^4 - 10(\omega\mathbf{p})^2 + 7\mathbf{p}^4$$

$$\Pi_q = p_x^2 p_y^2$$



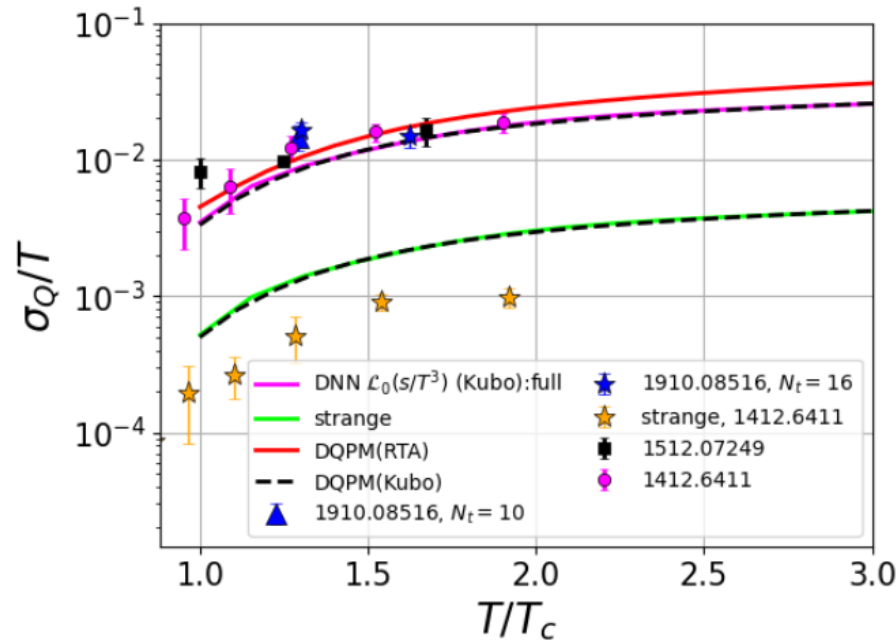
- Kubo formalism allows the evaluation of transport coefficients without involving estimations of cross-sections

# Conductivity: improve strange quark

Only quark sector

– separate strange sector

$$\sigma^{\text{Kubo}}(T) = \frac{1}{3T} \int \frac{d^4 p}{(2\pi)^4} \mathbf{p}^2 \sum_{i=a,\bar{a}} d_i ((1 \pm f_i(\omega)) f_i(\omega)) \rho_i(\omega, \mathbf{p})^2$$



- Conductivity shows how good we describe quark sector – we can compare to the **strange quark** conductivity
- Check how strangeness is described within the quasi-particle models and its influence on conductivity

# Generalization of QP Ansatz - Ag DNN Model

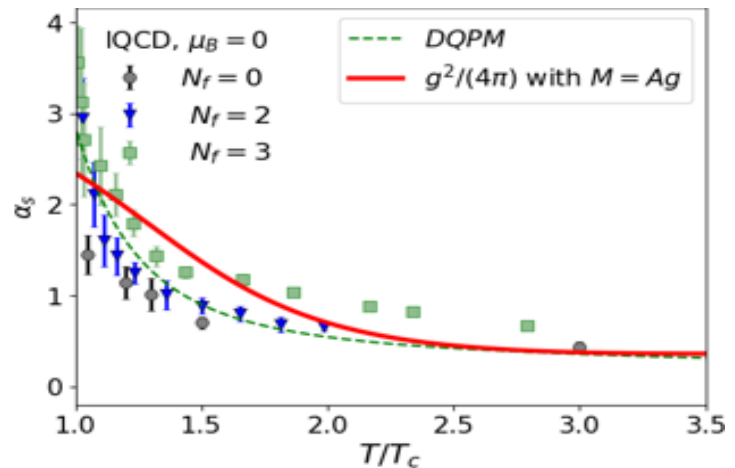
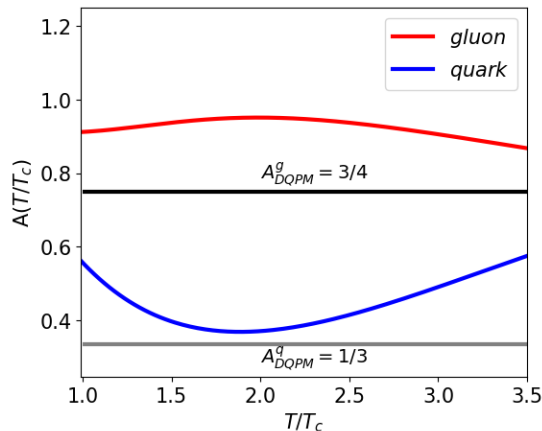
## Main ingredients

- 6 outputs (before just g)
- Modified loss function

$$\mathcal{L}_1 = \mathcal{L}_0 + \beta_{as}\mathcal{L}_{as} + \beta_{reg}\mathcal{L}_{DQPM}$$

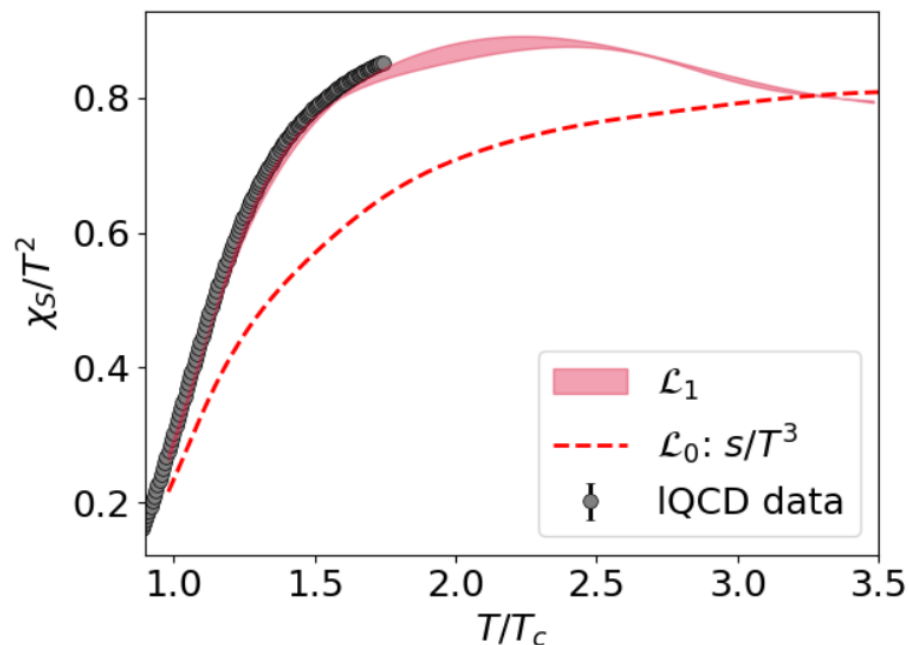
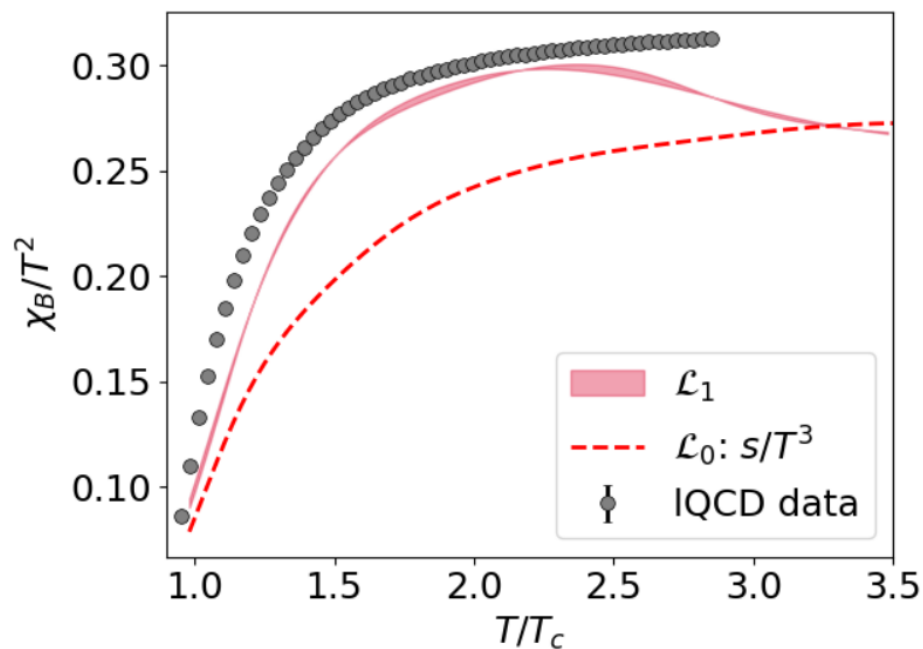
$$\mathcal{L}_{as} = \left[ \underline{\gamma}_l(T)/\underline{\gamma}_s(T) - 1 \right]^2 \quad |T > 2.5T_c$$

- No strict parametrization for widths
- Coupling constant extracted from the masses employing non perturbative corrections :  $\frac{m_{q/g}(T)}{T} = \underline{A}_{q/g}(T/T_c)\underline{g}(T/T_c)$



- Modification of strangeness

# Improved EoS from AgDNN

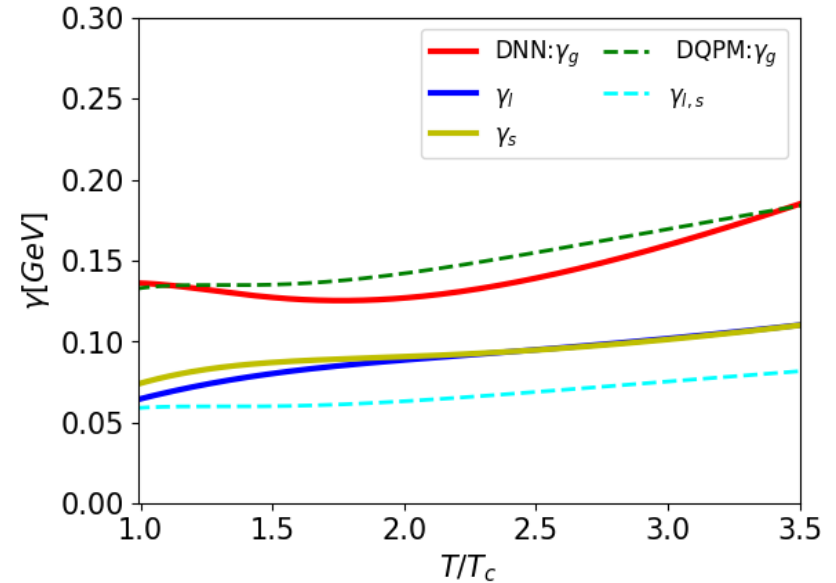
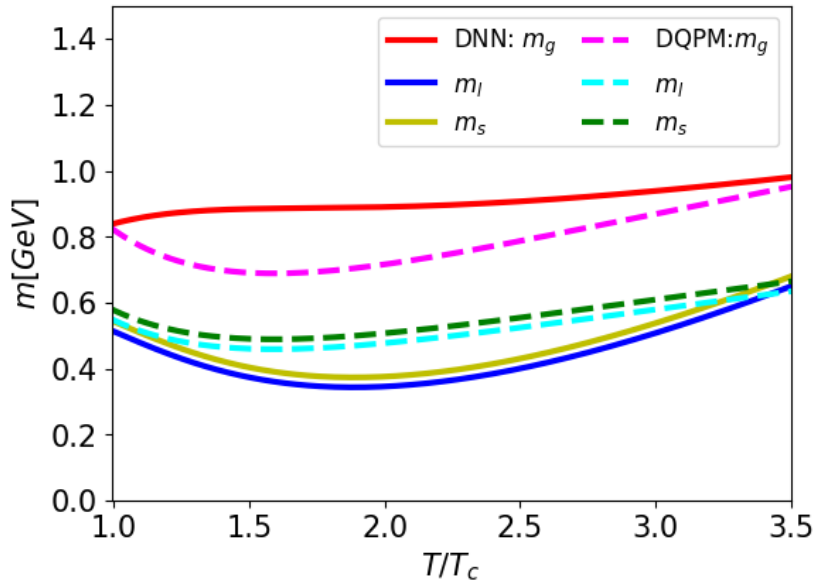


- Improved susceptibilities  $\chi_2^B(T), \chi_2^S(T)$
- Microscopic quantities have changed – but close to the original QDPM at  $3T_c$



# Microscopic properties from AgDNN

- Strangeness – simple shift  $m_{s(\bar{s})}(T) = m_{q(\bar{q})}(T) + \Delta m$

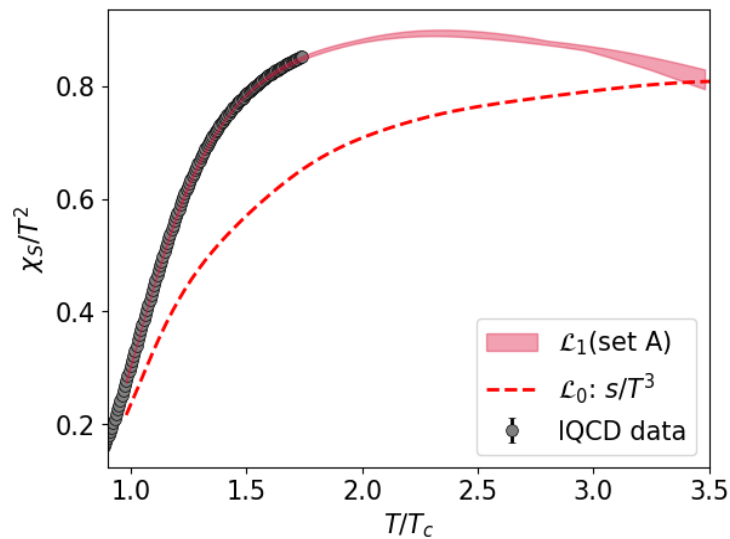
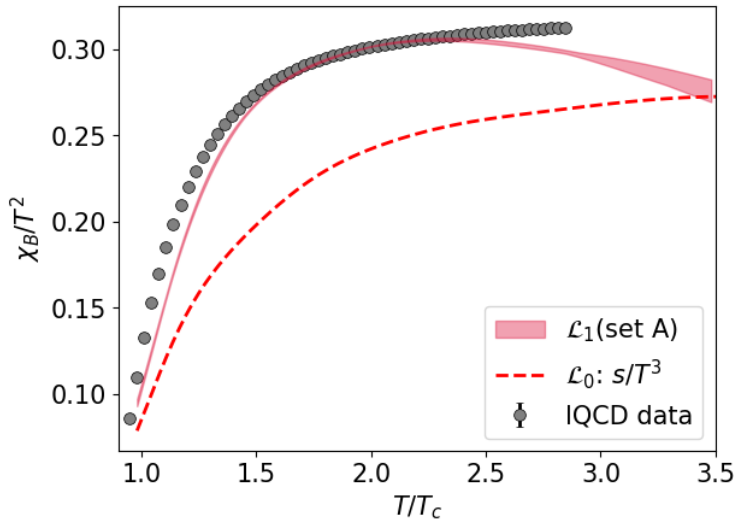


- Massive gluon shows – almost no  $T$  –dependence at small  $T < 3T_c$
- Smaller masses – but close to the original QDPM at  $3T_c$
- No constraints on widths at small  $T$  – only asymptotics

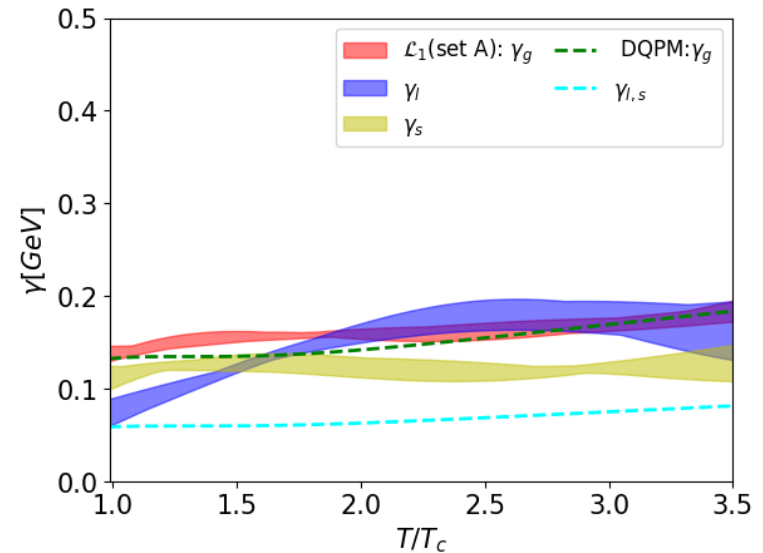
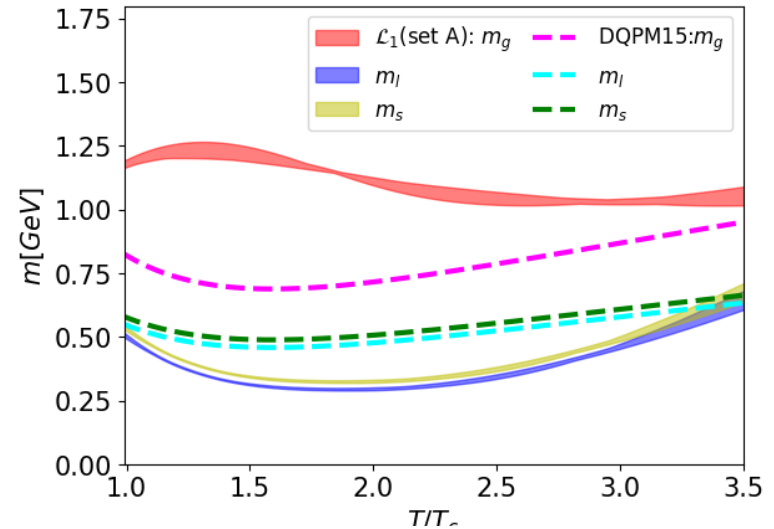
$$\mathcal{L}_{as} = \left[ \underline{\gamma}_l(T) / \underline{\gamma}_s(T) - 1 \right]^2 \Big|_{T > 2.5T_c}$$

# Microscopic properties from AgDNN

- Set A – higher susceptibilities

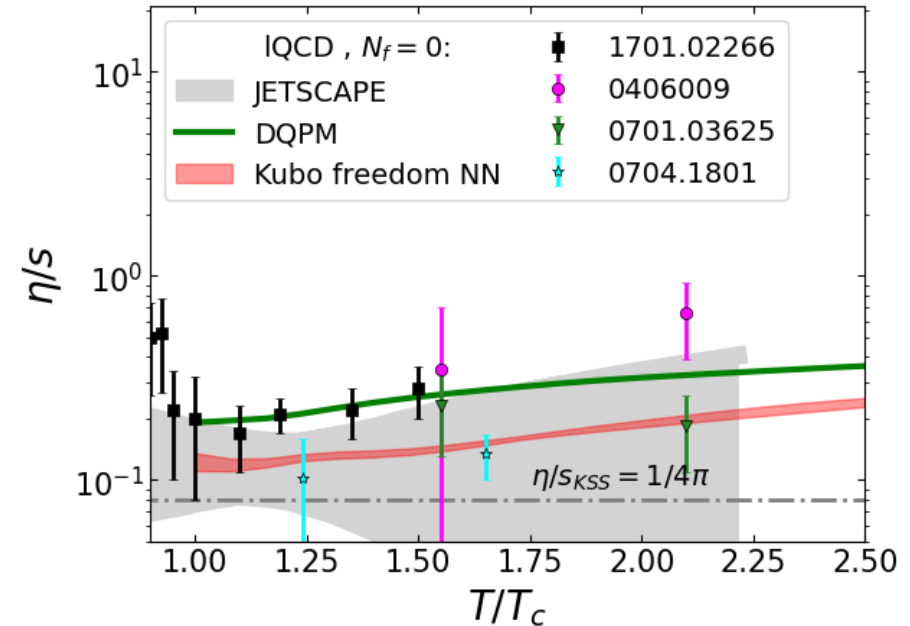
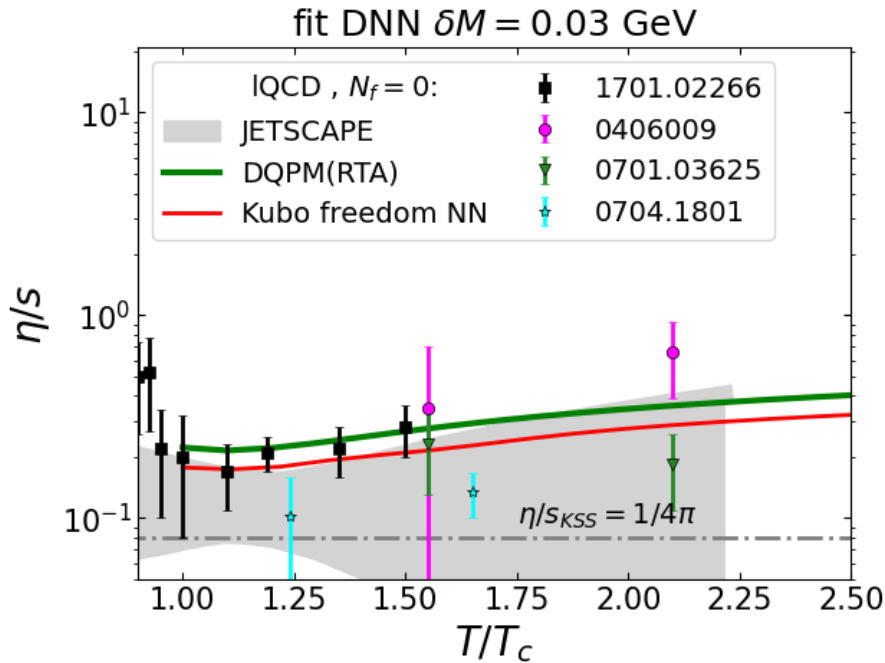


## heavy gluons:



# Transport coefficients from AgDNN

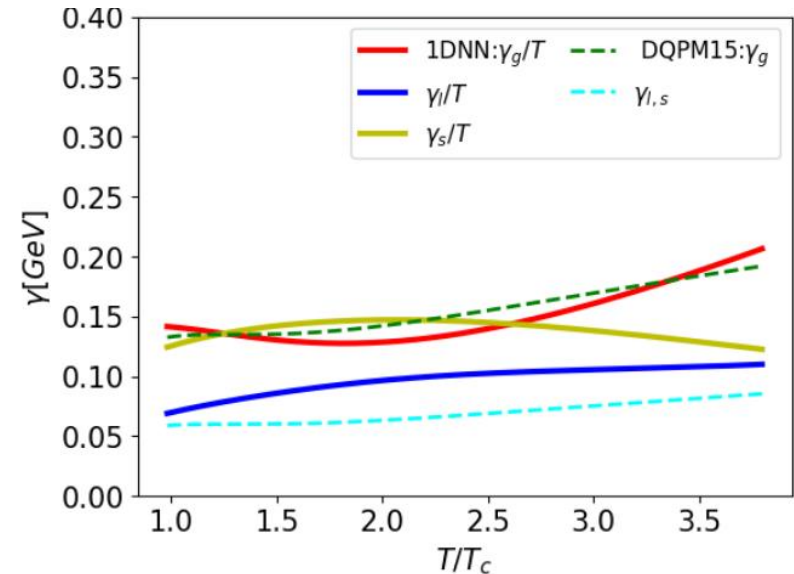
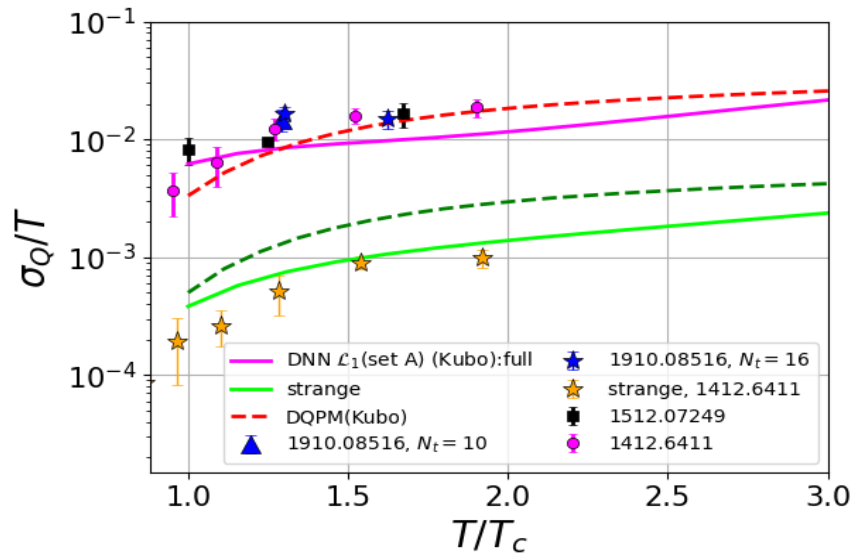
heavy gluons:



- Cross-check how good we describe the QGP: shear viscosity in a physical range
- Increase in gluon/light quark masses and widths affect the shear viscosity

# Tweak the strangeness – improve conductivity

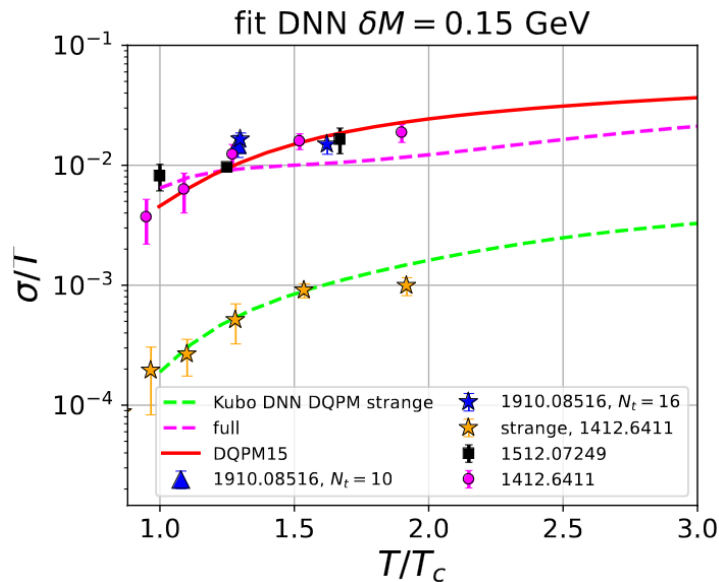
- Strangeness – higher widths



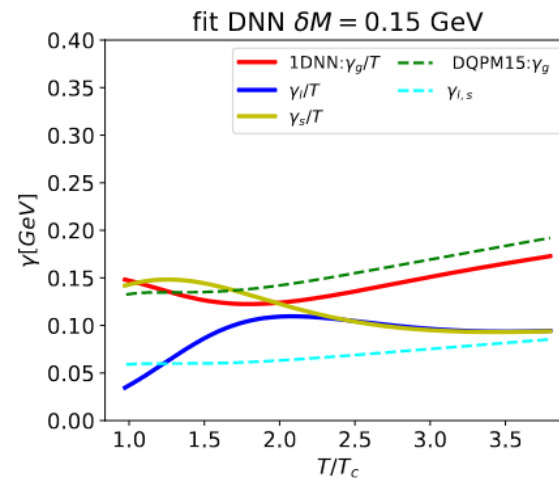
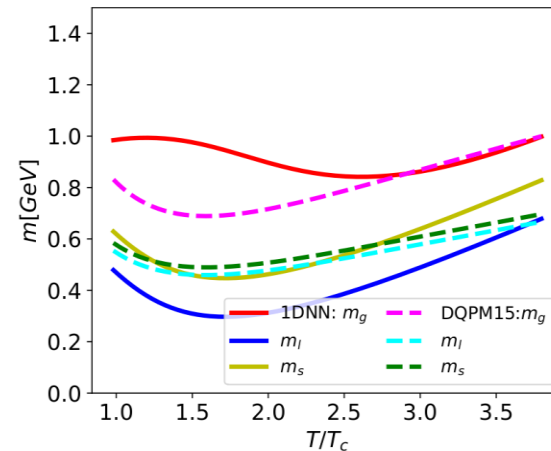
- Masses and widths of strange quark should differ from light sector
- DNN suggests higher widths and smaller masses compare to original parametrization

# Tweak the strangeness – improve conductivity

- Strangeness – simple shift



$$m_{s(\bar{s})}(T) = m_{q(\bar{q})}(T) + \Delta m$$



- DNN suggests higher widths and smaller masses compare to original parametrization, simple shift also works!
- 2 scenarios looks similar – we need more input from theory

# Summary

---

- We have created framework with small size NN to adjust model parameter (here quasi-particle description) microscopic properties of QGP phase using 3 thermodynamic quantities and transport coefficients (Kubo formalism)
- We found that effective masses/widths of strange quark should differ from the light quark to describe strange conductivity and susceptibility
- DNN can be useful for phenomenology only when regularization terms are provided
- Future application for other models – unsupervised learning can provide hints for the improvements of a model description

**Thank you for your attention!**

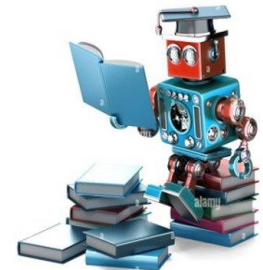
# Bonus: ML for HEP

Theory:

- Classify phases of matter - phase transitions in QCD
- **Exploring QCD matter in extreme conditions** with Machine Learning (recent review: <https://arxiv.org/abs/2303.15136>)

Jet flavour identification:

- › <https://arxiv.org/abs/1407.5675> - CNN, Josh Cogan et al;
- › <https://arxiv.org/abs/1603.09349> - DNN for jets, Pierre Baldi et al;
- › <https://arxiv.org/abs/1701.05927> - GAN for jets, Luke de Oliveira et al;
- › <https://arxiv.org/abs/1702.00748> - RNN for jets, Gilles Louppe et al;



And much more in

**Living Review of ML for Particle Physics ->**

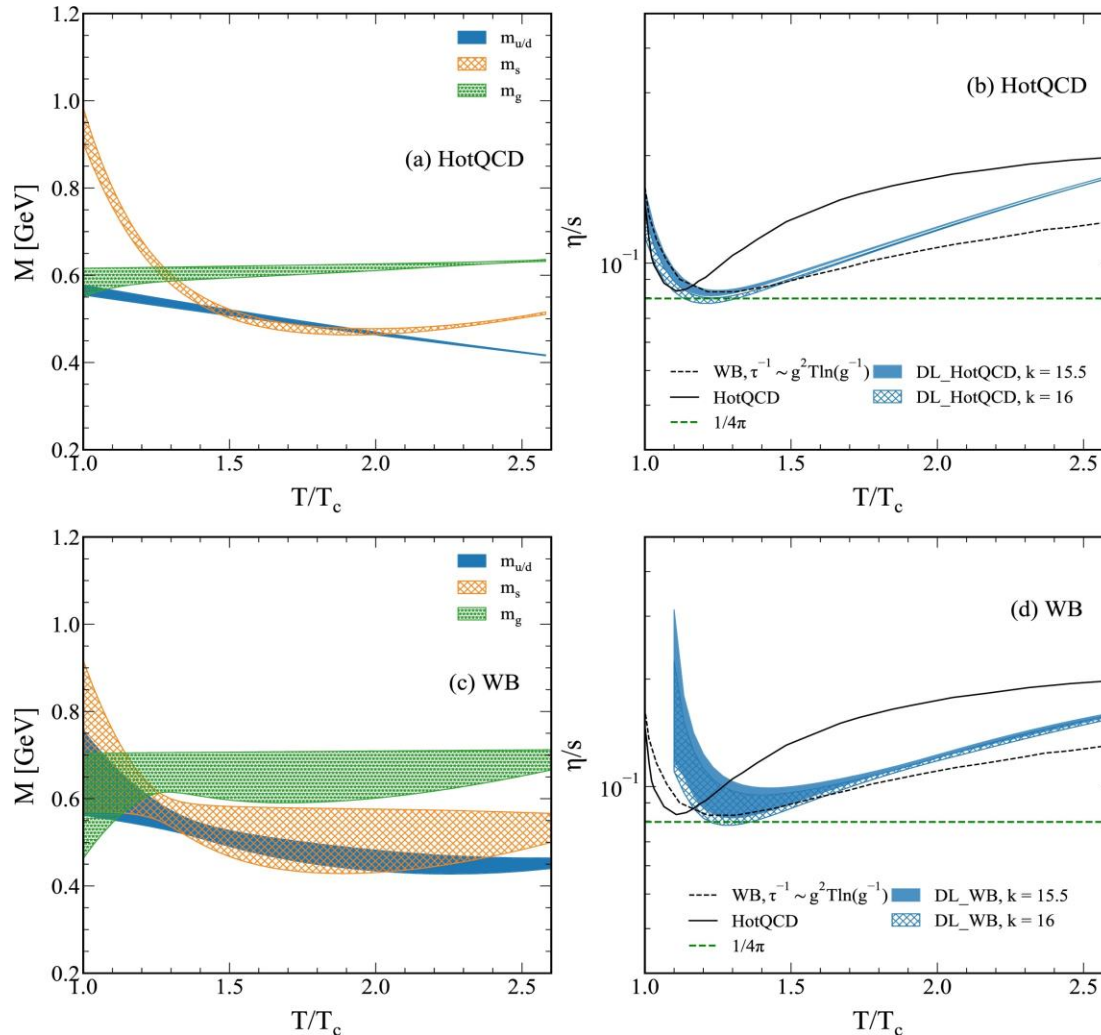
<https://github.com/iml-wg/HEPML-LivingReview>



**Thank you for your attention!**

# Comparison: on-shell results

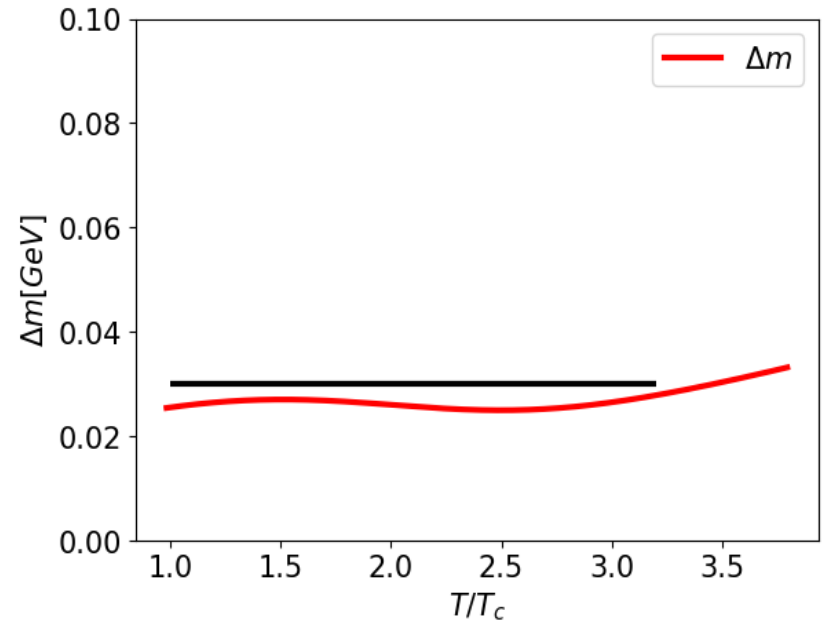
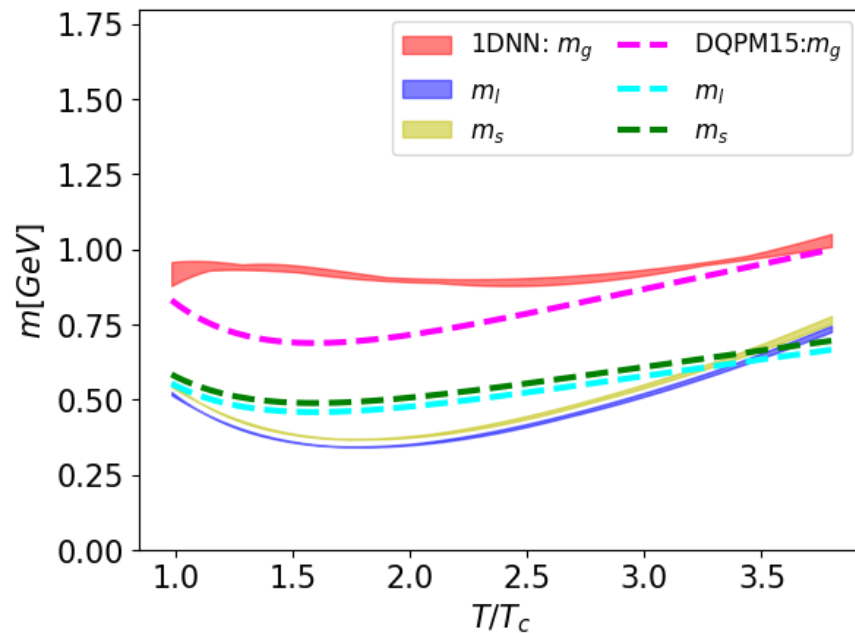
- 3 outputs – only masses – strong dependence on EoS





# Microscopic properties from AgDNN

- Strangeness – free parameter



- No constraints on strange quark mass/widths
- Original mass difference is preferable

# Framework: off-shell Quasi-Particle Model

$$\mathcal{L}_0 = \beta_G \left[ \frac{\tilde{s}(T) - s_{\text{IQCD}}}{\Delta s_{\text{IQCD}}} \right]^2 + \beta_L \left[ \frac{\tilde{\chi}^B(T) - \chi_{\text{IQCD}}^B}{\Delta \chi_{\text{IQCD}}^B} \right]^2 + \beta_S \left[ \frac{\tilde{\chi}^S(T) - \chi_{\text{IQCD}}^S}{\Delta \chi_{\text{IQCD}}^S} \right]^2$$

$$s(T) = -d_g I_g^B - d_q \sum_{i=q,s} I_i^F,$$

$$\chi_2^B(T) = \frac{d_q}{9} (2\chi_l(T) + \chi_s),$$

$$\chi_2^S(T) = d_q \chi_s,$$

$$I_i^B(T, m, \gamma) = \frac{1}{2\pi^2 T} \int d^3p \frac{4p^2 + 3m_i^2}{3\sqrt{\omega^2 + p^2}} f_B(\omega, T) + 2 \int_0^\infty \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} \frac{\partial f_B(\omega, T)}{\partial T} h(\omega, p, m_i, \gamma_i),$$

$$I_i^F(T, m, \gamma) = \frac{1}{2\pi^2 T} \int d^3p \frac{4p^2 + 3m_i^2}{3\sqrt{\omega^2 + p^2}} f_F(\omega, T) + 2 \int_0^\infty \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} \frac{\partial f_F(\omega, T)}{\partial T} h(\omega, p, m_i, \gamma_i),$$

$$\chi_i(T, m, \gamma) = \frac{1}{2\pi^2 T} \int_0^\infty dp \frac{p^2}{1 + \cosh\left(\frac{\sqrt{m_i^2 + p^2}}{T}\right)} + 2 \int_0^\infty \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} \frac{\sinh(\omega/T)}{T^2 (1 + \cosh(\omega/T))^2} h(\omega, p, m_i, \gamma_i)$$

# How to evaluate transport coefficient?

- **Kubo formalism: transport coefficients are expressed through correlation functions of stress-energy tensor**

used in lattice QCD, transport approaches(hadrons), effective models

$$\eta = \frac{1}{20} \lim_{\omega \rightarrow 0} \frac{1}{\omega} \int d^4x e^{i\omega t} \langle [S^{ij}(t, \mathbf{x}), S^{ij}(0, \mathbf{0})] \rangle \theta(t) \quad S^{ij} = T^{ij} - \delta^{ij} \mathcal{P}$$

$$\zeta = \frac{1}{2} \lim_{\omega \rightarrow 0} \frac{1}{\omega} \int d^4x e^{i\omega t} \langle [\mathcal{P}(t, \mathbf{x}), \mathcal{P}(0, \mathbf{0})] \rangle \theta(t) \quad \mathcal{P} = -\frac{1}{3} T^i_i$$

R. Lang and W. Weise, EPJ. A 50, 63 (2014) (NJL model)

A. Harutyunyan et al, PRD 95, 114021, (2017)

## Kinetic theory:

- **Relaxation time approximation(RTA): consider relaxation time**  $\frac{df_a^{\text{eq}}}{dt} = C_a = -\frac{f_a^{\text{eq}} \phi_a}{\tau_a}$ 

P. Chakraborty and J. I. Kapusta, PRC 83,014906 (2011)  
G.S. Rocha, M. N. Ferreira, G. S. Denicol and J. Noronha, PRD 106 (2022) no.3, 036022
- **Chapman-Enskog: expand the distribution in terms of the Knudsen number**

J. A. Fotakis et al, PRD 101 (2020) 7, 076007 (HRG)

## And more!

## Holographic models: AdS/CFT correspondence

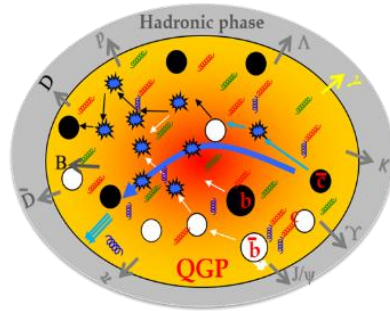
D. T. Son and A. O. Starinets, JHEP 0603, 052 (2006)

M. Attems et al, JHEP 10 (2016), 155.

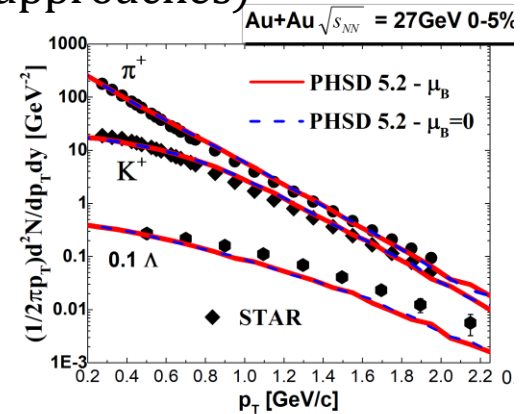
J. Grefa, M. Hippert, J. Noronha, J. Noronha-Hostler, I. Portillo, C. Ratti and R. Rougemont, PRD 106 (2022) no.3, 034024 <- near CEP and across the first-order line

# Properties of QGP: transport coefficients

! One has to specify transport and microscopic properties as well as EoS for theoretical simulations of HICs (hydro / transport approaches)



Evolution of QCD medium



## Hybrid simulations:

vHLE/Music+UrQMD/SMASH

Iu.A. Karpenko, P. Huovinen, H. Petersen and M. Bleicher

PRC 91 (2015), 064901.

CORE-CORONA – EPOS (K. Werner), DCCI(Y. Kanakuba)

MUFFIN

## Transport simulations with QGP phase:

Catania transport – QuasiParticle Model

F. Scardina, S. K. Das, V. Minissale, S. Plumari, and V. Greco,

PRC 96, 044905 (2017).

AMPT – PNJL EoS (Mean field potentials)

K.J. Sun, C. M. Ko, and Z.-W. Lin, PRC 103(2021)



– off-shell transport approach derived from Kadanoff-Baym many-body theory (Quantum Boltzmann) with hadronic and QGP phase – 2PI Dynamical QuasiParticle Model

W. Cassing, E. Bratkovskaya, PRC 78 (2008) 034919

P. Moreau, O. S, L. Oliva, T. Song, W. Cassing, E. Bratkovskaya, PRC 100 (2019), 014911;

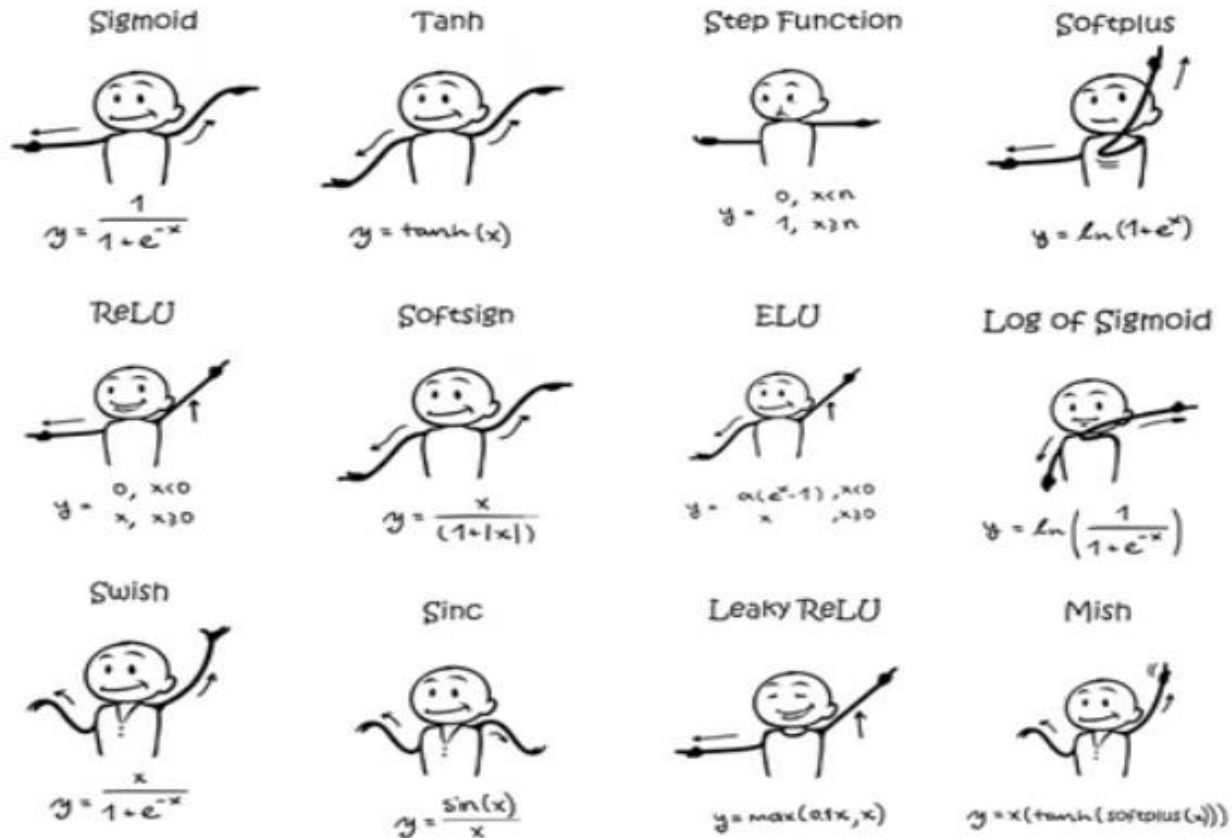
O. S, P. Moreau, L. Oliva, V. Voronyuk, V. Kireyeu, T. Song, E. Bratkovskaya, Particles 3 (2020)

# Machine Learning: Basic concepts

$$h = \Theta\left(\sum w_i x_i + b\right)$$

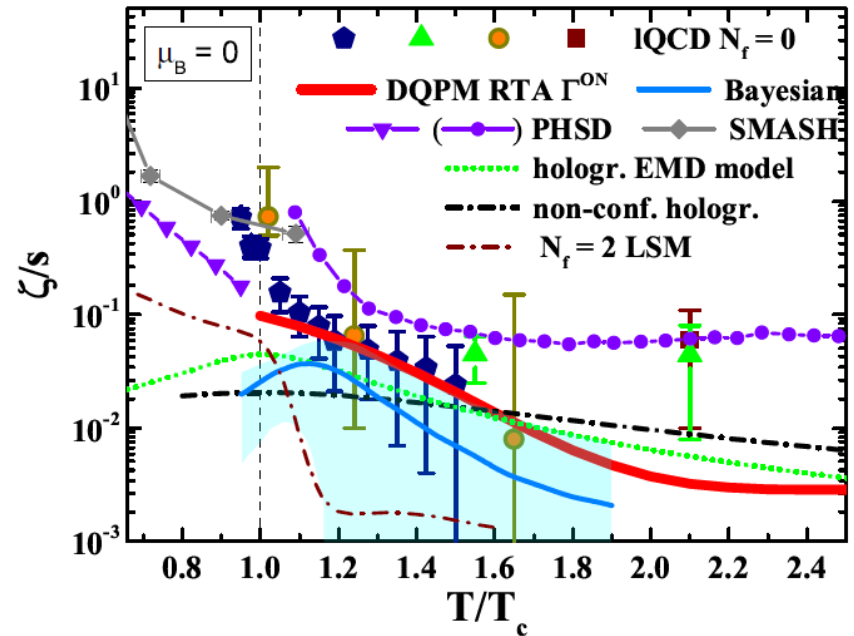
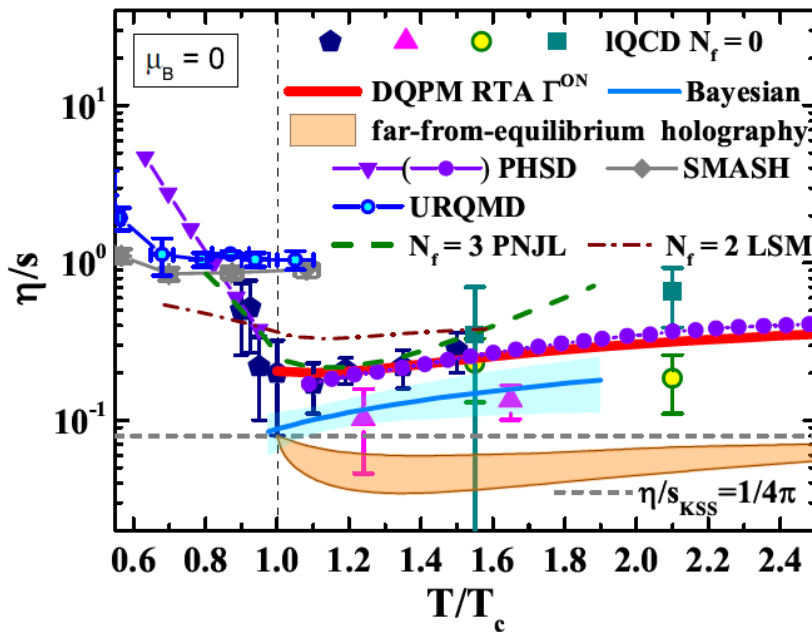
- ›  $\Theta(x)$  — Heaviside function  
(0, if  $x \leq 0$ , 1 otherwise)
- › non-smooth  $\Rightarrow$  hard to optimize

Alternatives: choose wisely!



# Uncertainties in viscosities of QGP

Model predictions: from first principles to effective models – quest for consistency



**!** Effective models of QGP using the same EoS predict completely different transport coefficients

# Machine Learning: Unsupervised

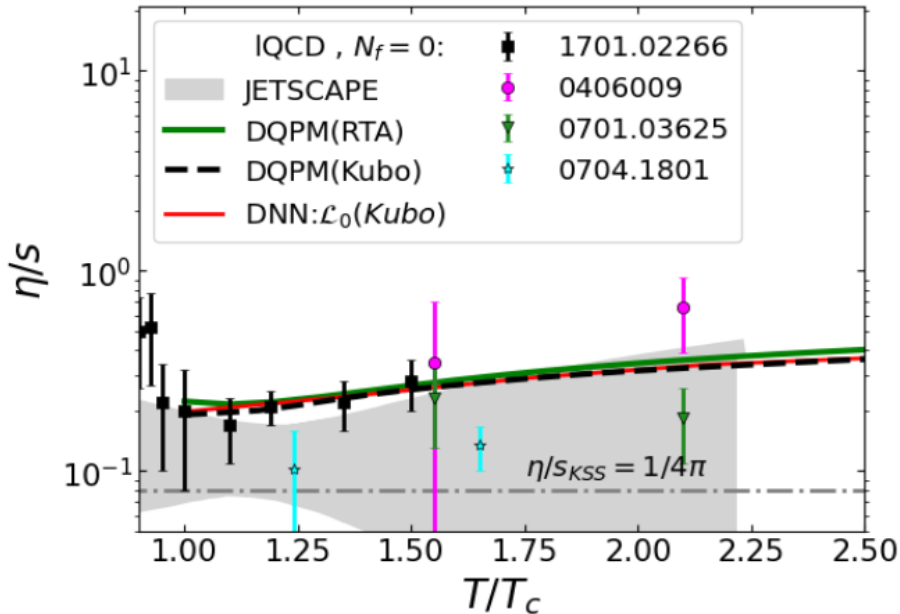
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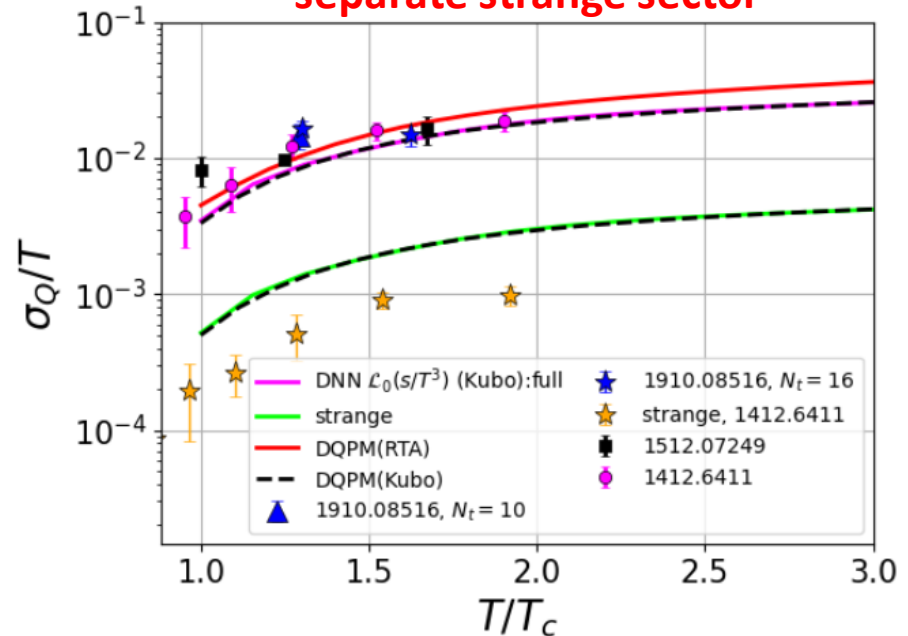
- Unsupervised Learning is most promising/suitable for phenomenology and physics

# Strange conductivity: reconsider strange quark

Contain all degrees of freedom



Only quark sector  
– separate strange sector



- Kubo formalism allows to evaluate transport coefficients without involving cross-sections
- Conductivity shows how good we describe quark sector – in particular we can compare to the **strange quark** conductivity
- Check how strangeness is described within the quasi-particle models and its influence on conductivity