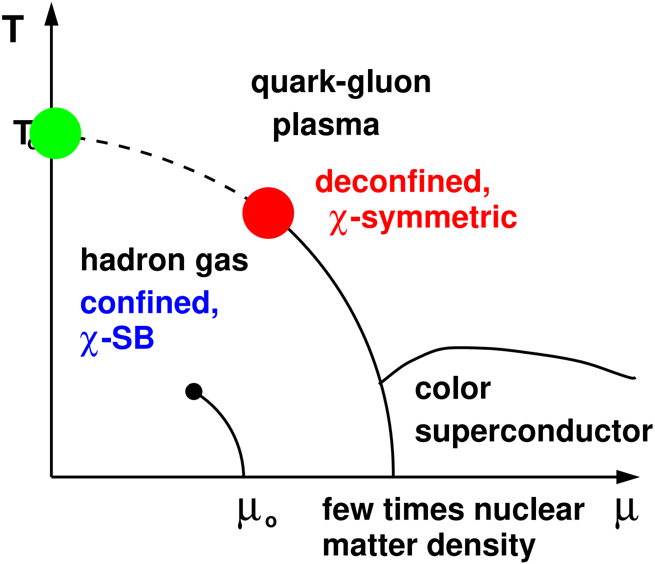
Quarkonium in Non-Zero Temperature from Lattice NRQCD

Seyong Kim

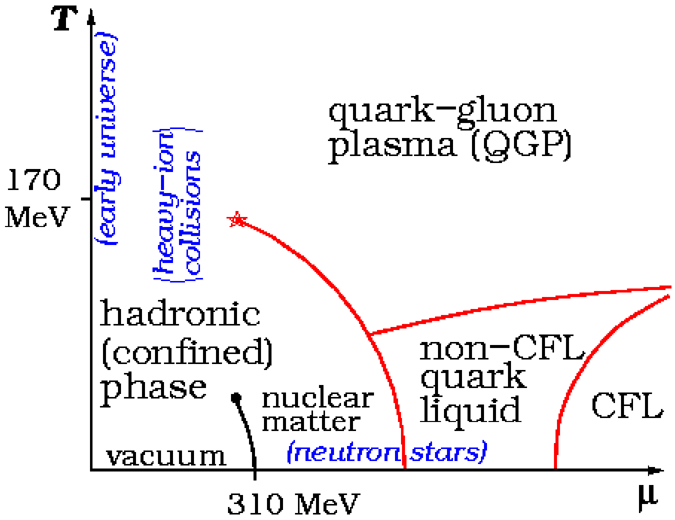
Sejong University

Outline

QCD phase diagram

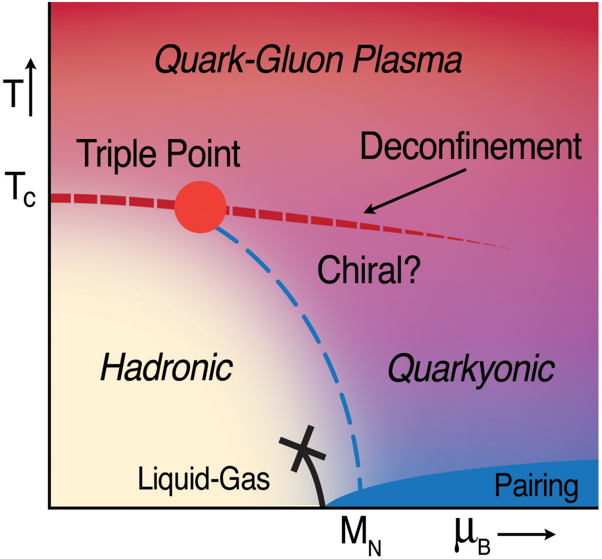


QCD phase diagram



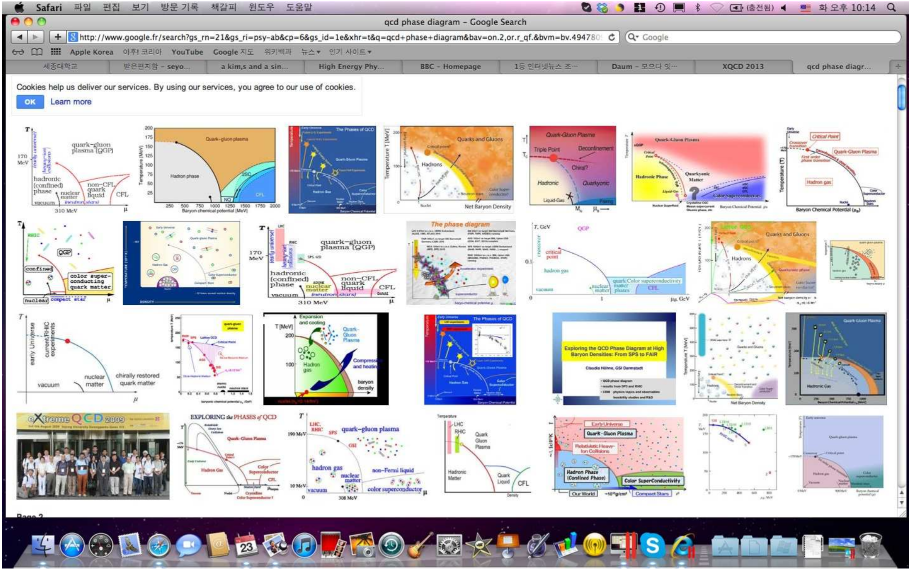
from Wikipedia

QCD phase diagram



from arXiv:0911.4806

QCD phase diagram



Why Lattice?

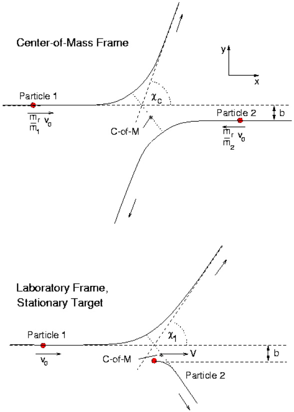
What's the most central quantity

in high energy nuclear/particle physcs ?

Why Lattice?

Differential Cross Section

- the probability to find a particle with energy E and the momentum $\vec{p}$



(silas.psfc.mit.edu)

Why Lattice?

• experimentally count the number of particles with energy E and the momentum $\vec{p}$ / total number of collisions

• theoretically compute the probability for a particle with energy E and the momentum $\vec{p}$ after a collision

Why Lattice?

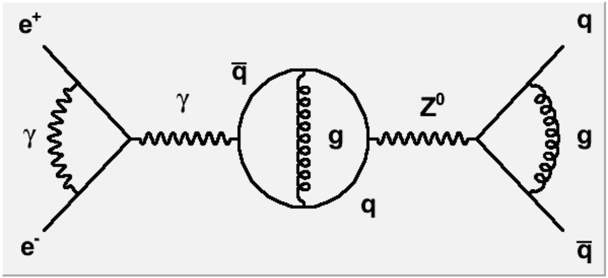
$$d\Gamma(a \to 1234\cdots) = \frac{1}{2E_a}|\langle 1234\cdots|\hat{T}^\dagger|a\rangle|^2$$
$$\times(2\pi)^4\delta^4(P_a - \sum_{i=1}^{N} P_i)\prod_{i=1}^{N}\frac{d^3p_i}{2E_i(2\pi)^3}$$

$$d\sigma(a+b \to 1234\cdots) = \frac{1}{4\sqrt{(E_aE_b - \mathbf{p}_a\cdot\mathbf{p}_b)^2 - m_a^2m_b^2}}|\langle 1234\cdots|\hat{T}^\dagger|ab\rangle|^2$$
$$\times(2\pi)^4\delta^4(P_a + P_b - \sum_{i=1}^{N} P_i)\prod_{i=1}^{N}\frac{d^3p_i}{2E_i(2\pi)^3}$$

• differential cross section = normalization factor × matrix element square × phase space

• Feynman rules: theorists' method to construct matrix elements and compute cross sections for weakly interacting cases

Why Lattice?



Why Lattice?

What if the interaction is strong?

Path integral formulation

What do we need to calculate?

$$|\text{matrix element}|^2 = |\langle 123 \cdots | \hat{T}^\dagger | ab \rangle|^2$$

and spectrum (particle masses)

Path integral formulation

• In quantum mechanics ((0+1)-dimensional quantum field theory), solve

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = \hat{H}\psi(\mathbf{x},t)$$

and calculate

$$\langle\psi_f|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\psi_i\rangle$$

• interaction picture and perturbation theory

$$\hat{H} = \hat{H}_0 + \hat{H}_{\rm int}$$

Path integral formulation

- consider

$$
\begin{aligned}
&\langle \psi_f(t_f)|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\psi_i(t_i)\rangle \\
=&\langle \psi_f(t_f)|\int d^3\,x|\mathbf{x}\rangle\langle \mathbf{x}e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\int d^3\,x'|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi_i(t_i)\rangle \\
=&\int d^3\,x\int d^3\,x'\psi_f(\mathbf{x},t_f)^\dagger\psi_i(\mathbf{x}',t_i)\langle \mathbf{x}|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\mathbf{x}'\rangle
\end{aligned}
$$

- and Green function method

$$
G(\mathbf{x},t_f|\mathbf{x}',t_i)=\langle \mathbf{x}|e^{-\frac{i}{\hbar}\hat{H}(t_f-t_i)}|\mathbf{x}'\rangle,
$$

and

$$
\psi_f(\mathbf{x},t_f)=\int d^3x'G(\mathbf{x},t_f|\mathbf{x}',t_i)\psi_i(\mathbf{x}',t_i)
$$

Path integral formulation

$$G(x,t_f|x',t_i) = \langle x|e^{-i\hat{H}T}|x'\rangle$$
$$= \int dx_N \langle x|e^{-i\hat{H}\varepsilon}|x_N\rangle\langle x_N|e^{-i\hat{H}\varepsilon}\int dx_{N-1}|x_{N-1}\rangle\langle x_{N-1}|e^{-i\hat{H}\varepsilon}\cdots$$
$$\times \int dx_1|x_1\rangle\langle x_1|e^{-i\hat{H}\varepsilon}|x'\rangle$$

where $\varepsilon = \frac{T}{N}$.

- insert $\int dp_i|p_i\rangle\langle p_i|$

$$\langle x_i|e^{-i\varepsilon\hat{H}}|x_{i-1}\rangle = \int dp_i \langle x_i|p_i\rangle\langle p_i|e^{-i\varepsilon\hat{H}}|x_{i-1}\rangle$$
$$\sim \int dp_i \langle x_i|p_i\rangle e^{-i\varepsilon\left[\frac{p_i^2}{2m}+V(x_{i-1})\right]}\langle p_i|x_{i-1}\rangle$$
$$\sim \int dp_i e^{-i\left[p_i(x_{i-1}-x_i)+\varepsilon\frac{p_i^2}{2m}+\varepsilon V(x_{i-1})\right]} \sim e^{-i\varepsilon\left[\frac{1}{2}m\left(\frac{x_i-x_{i-1}}{\varepsilon}\right)^2-V(x_{i-1})\right]}$$

Path integral formulation

$$G(x,t_f|x',t_i) = \langle x|e^{-i\hat{H}T}|x'\rangle = \int \prod_{i=1}^{N} dx_i e^{-i\varepsilon \sum_i L(t_i)} = \int \mathcal{D}x(t) e^{-iS},$$

and

$$S = \int_{t_i}^{t_f} dt\, L[x(t)] = \int_{t_i}^{t_f} dt \left[\frac{1}{2} m \left(\frac{dx}{dt}\right)^2 - V(x(t))\right]$$

Statistical mechanics

- partition function

$$Z = \mathrm{Tr}\left(e^{-\frac{\hat{H}}{k_B T}}\right) = \sum_n e^{-\frac{E_n}{k_B T}} = \int d\,x \langle x | e^{-\frac{\hat{H}}{k_B T}} | x \rangle$$

With $k_B = 1$ and $\hbar = 1$ and $\tau_f - \tau_i = \frac{1}{T}$ and the periodic boundary condition,

$$Z = \int \mathcal{D}x(\tau) e^{-S},$$

and

$$S = \int_{\tau_i}^{\tau_f} d\,\tau \left[\frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2 + V(x(\tau))\right],$$

- Euclidean space ($it \to \tau$) and statistical mechanics

Statistical mechanics

Quantum mechanics problem is a statistical mechanics problem

cf. M. Creutz and B. Freedman, “A statistical approach to quantum mechanics”, Annals. Phys. 132 (1981) 427.

- generalization to field theory

Statistical mechanics

Green function is a correlation function in a statistical mechanics setup

Statistical mechanics

- two point function (two point Green function) or two point correlation function

$$\langle 0|\hat{x}(\tau)\hat{x}(0)|0\rangle = \langle 0|e^{\tau\hat{H}}\hat{x}(0)e^{-\tau\hat{H}}\hat{x}(0)|0\rangle$$

$$= \sum_n |\langle 0|\hat{x}(x)|n\rangle|^2 e^{-E_n\tau}$$

- and 3-point, 4-point functions or more.

Lattice gauge theory

$$< O >= \frac{\int d\psi(x) d\overline{\psi(x)} dA_\mu(x) e^{-(S_g+S_f)/\hbar} O}{\int d\psi(x) d\overline{\psi(x)} dA_\mu(x) e^{-(S_g+S_f)/\hbar}}$$

where $S_g = -\frac{1}{4} F^a_{\mu\nu} F^{\mu\nu a}(x), S_f = \overline{\psi}(x)(\gamma_\mu D_\mu + m)\psi(x)$

$F^a_{\mu\nu} T^a = \partial_\mu A^a_\nu T^a - \partial_\nu A^a_\mu T^a + ig[A^b_\mu T^b, A^c_\nu T^c]$

$[T^b, T^c] = if_{bca} T^a$ (T^a : Gell-Mann matrices, generator for SU(3) group

and $D_\mu \psi(x) = (\partial_\mu - igA^a_\mu T^a)\psi(x)$.

- infinite dimensional integral problem

- numerical integration – Monte-Carlo method

Lattice gauge theory

- general Monte-Carlo algorithm

$$< \mathcal{O} >= \frac{\int d\psi(x) d\overline{\psi(x)} dA_\mu(x) e^{-(S_g+S_f)} \mathcal{O}}{\int d\psi(x) d\overline{\psi(x)} dA_\mu(x) e^{-(S_g+S_f)}}$$

$$\rightarrow \frac{\int dA_\mu(x) e^{-S_g} \mathrm{Det}(\gamma_\mu D_\mu + m) \mathcal{O}(A_\mu, (\gamma_\mu D_\mu + m)^{-1})}{\int dA_\mu(x) e^{-S_g} \mathrm{Det}(\gamma_\mu D_\mu + m)}$$

$$\rightarrow \frac{\int dA_\mu(x) e^{-S_g} \mathcal{O}(A_\mu, (\gamma_\mu D_\mu + m)^{-1})}{\int dA_\mu(x) e^{-S_g}}$$

- Grassmann variable integraion

$$< \mathcal{O} >\sim \int dA_\mu \mathcal{P}(A_\mu) \mathcal{O}(A_\mu, (\gamma_\mu D_\mu + m)^{-1})$$

- generate A_μ which satisfies the above probability interpretation.

$$< \mathcal{O} >\sim \frac{1}{N} \sum_{i=N_0}^{N_0+N} \mathcal{O}(A_\mu^i)$$

Lattice gauge theory

- importance sampling

- detailed balance : choose $P(C', C)$ such that

$$P(C', C)e^{-\beta S(c)} = P(C, C')e^{-\beta S(C')}$$

- public code: MILC, OpenQCD, Chroma and etc

- temperature is defined as the inverse of the Euclidean time extent

- periodic boundary condition on bosonic field, anti-periodic boundary condition on fermionic field

Lattice gauge theory

- three steps for lattice gauge theory

1. generate set of field configurations
2. compute observables O using this set
3. analysis of computed observables
   and necessary analytic calculations
   (continuum extrapolation, renormalization, matching ...)

Heavy quark/quarkonium on a lattice

- free parameters:

  quark masses (u,d,s), bare gauge coupling constant,
  number of quark flavors

- physical quark mass

- continuum limit (lattice spacing, $a \to 0$ limit)

- large enough space ($V = (N_s a_s)^3$)

- computer doesn't know dimensional quantities

  everything expressed in terms of lattice spacing
  e.g., ρ meson mass is # $\times a^{-1}$

Heavy quark/quarkonium on a lattice

• if simulation done with light quark masses somewhat larger than physical u, d, s quark mass

$\rightarrow$ need extrapolation

• simulation done with $a \neq 0$

$\rightarrow$ scaling violation, need to check

• computer power limit no. of degrees freedom

$\rightarrow$ physical volume is limited, need to check

• $\frac{1}{M} > a$ for heavy quark • for heavy quark, the lattice spacing should

be small enough and the number of lattice sites becomes larger for a fixed physical volume

Heavy quark/quarkonium on a lattice

- temperature is defined as $T = \frac{1}{N_\tau a}$

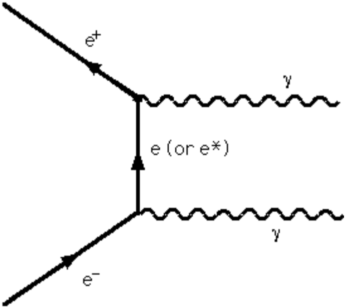
  $\leftarrow$ a is controlled by gauge coupling constant
  $\leftarrow$ different temperature means a different gauge coupling constant

- no. of spatial lattice sites (N_s) is usually bigger than N_τ

- $Ma > 1$: effective field theory

NRQCD Basics

- annihilation cross-section



NRQCD Basics

- relativity + quantum theory = quantum field theory

$$\mathcal{L} = \overline{\psi}(\not{D} + m)\psi - \frac{1}{4}F_{\mu\nu}F_{\mu\nu}$$

- but we are familiar with quantum mechanics !

$$i\,\not{h}\frac{\partial\phi}{\partial t} = \mathcal{H}\phi$$

- how do we go from a relativistic quantum field theory to quantum mechanics ?

NRQCD Basics

• do you remember relativistic quantum mechanics? and how to derive hyperfine interaction and etc?

• in Coulomb gauge, Foldy-Wouthuysen-Tani transform

• in field theory language, NRQCD is an effective theory in which the momentum mode higher than the heavy quark mass, M, is integrated away

• need to show power-counting and factorization etc (cf. Braaten, Bodwin, Lepage, Phys. Rev. D51 (1995) 1125)

• inclusive decay rate = partonic decay rate $\times$ the probability for heavy quark to meet anti-heavy quark

• long distance ME can be calculated by lattice method (e.g, Bodwin, Sinclair, Kim, PRL77 (1996) 2376)

NRQCD Basics

• scale separation: $M >> Mv >> Mv^2$

• the momentum scale larger than M is integrated out

• the distribution of heavy quark in the rest frame of quarkonium is determined by bound state dynamics (Mv)

NRQCD Basics

$$\mathcal{L} = \mathcal{L}_0 + \delta\mathcal{L}, \tag{1}$$

with

$$\mathcal{L}_0 = \psi^\dagger \left(D_\tau - \frac{\mathbf{D}^2}{2M} \right) \psi + \chi^\dagger \left(D_\tau + \frac{\mathbf{D}^2}{2M} \right) \chi, \tag{2}$$

and

$$\begin{aligned}
\delta\mathcal{L} = \quad & -\frac{c_1}{8M^3} \left[\psi^\dagger (\mathbf{D}^2)^2 \psi - \chi^\dagger (\mathbf{D}^2)^2 \chi \right] \\
& + c_2 \frac{ig}{8M^2} \left[\psi^\dagger \left(\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} \right) \psi + \chi^\dagger \left(\mathbf{D} \cdot \mathbf{E} - \mathbf{E} \cdot \mathbf{D} \right) \chi \right] \\
& - c_3 \frac{g}{8M^2} \left[\psi^\dagger \sigma \cdot (\mathbf{D} \times \mathbf{E} - \mathbf{E} \times \mathbf{D}) \psi + \chi^\dagger \sigma \cdot (\mathbf{D} \times \mathbf{E} - \mathbf{E} \times \mathbf{D}) \chi \right] \\
& c_4 \frac{g}{2M} \left[\psi^\dagger \sigma \cdot \mathbf{B} \psi - \chi^\dagger \sigma \cdot \mathbf{B} \chi \right].
\end{aligned} \tag{3}$$

NRQCD Basics

- lattice NRQCD at $T = 0$ is well established: 2012 PDG summary on QCD

28 *9. Quantum chromodynamics*

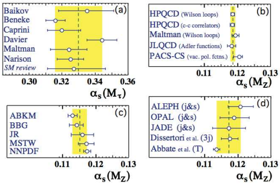
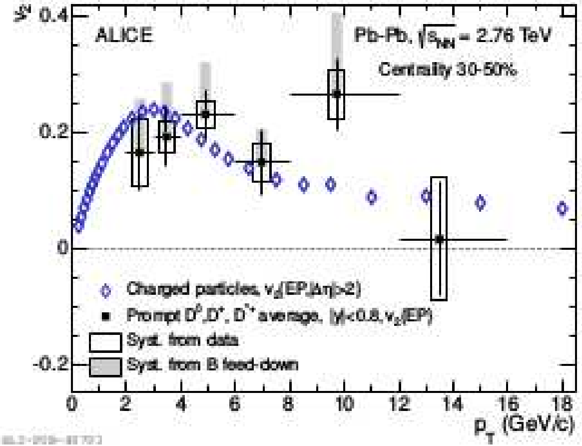


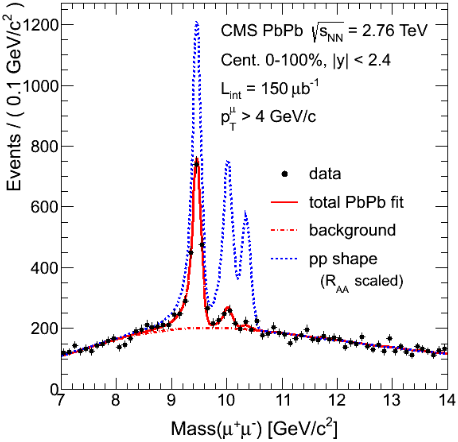
Figure 9.2: Summary of determinations of α_s from hadronic τ-decays (a), from lattice calculations (b), from DIS structure functions (c) and from event shapes and jet production in e^+e^--annihilation (d). The shaded bands indicate the average values chosen to be included in the determination of the new world average of α_s.

NRQCD Basics



- elliptic flow (v_2) of $D-$meson: ALICE, PRC 90 (2014) 034904

NRQCD Basics



- sequential suppression of $\Upsilon(1S, 2S, 3S)$: CMS, PRL109 (2012) 222301

NRQCD Basics

• Investigation of QGP properties requires comparison between the baseline (p, p) and relativistic heavy ion collisions

• heavy quark system is one of better understood hadronic systems

• heavy quark mass scale(M) is large and the strong coupling at the mass scale is “small”

$\rightarrow$ separation of bound state dynamics from short distance perturbative dynamics

•effective field theory descriptions : NRQCD (pNRQCD), HQET (cf. G.T.Bodwin, E. Braaten, G.P. Legage, PRD51 (1995) 1125, N. Brambilla, A. Pineda, J. Soto, and A. Vairo, Rev. Mod. Phys 77 (2005) 1423, N. Isgur and M. Wise, PLB 237 (1990) 527)

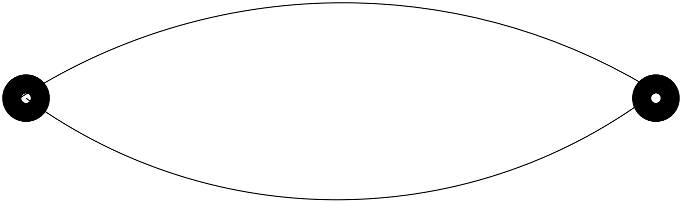
• with $T << M$, EFT still in operation (?)

NRQCD Basics

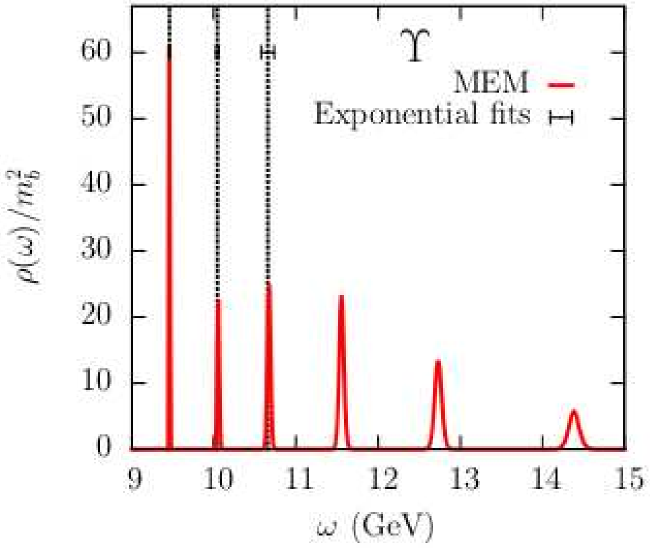
1. direct simulation of relativistic heavy quark system on lattice is difficult due to wide scale separations (confinement, heavy quark de Broglie wavelength, light quark de Broglie wavelength, lattice cutt-off)
2. calculating real time quantities using Euclidean lattices is diffcult
3. spectral behavior in non-zero temperature is more complex than the zero temperature case (thermal broadening, transport phenomena, disappearance of bound states, and etc)

NRQCD Basics

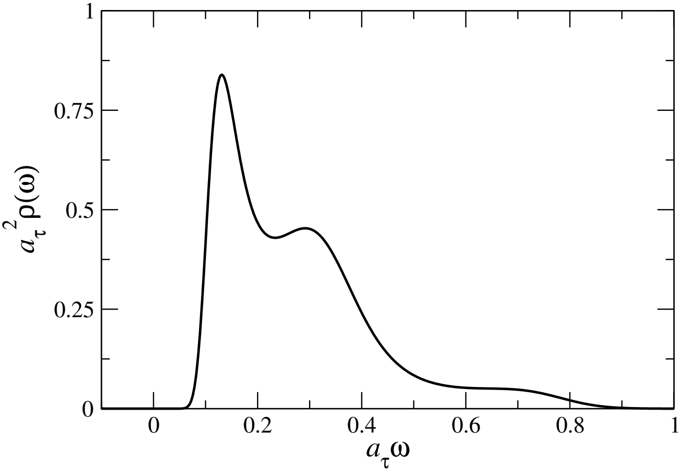
$$G(\tau) = \sum_{\vec{x}} G_Q(\vec{x}, \tau : \mathbf{0}, 0) G_Q(\vec{x}, \tau : \mathbf{0}, 0)^{\dagger}$$



NRQCD Basics



NRQCD Basics



$$G(\tau) = A_0 e^{-E_0 \tau} + A_1 e^{-E_1 \tau} + \cdots \qquad \text{vs.} \qquad = \int \frac{d\omega}{2\pi} K(\tau, \omega)\, \rho(\omega)$$

NRQCD Basics

• obtaining spectral function from Euclidean correlators which is defined in terms of integral equation is numerically "ill-posed problem"

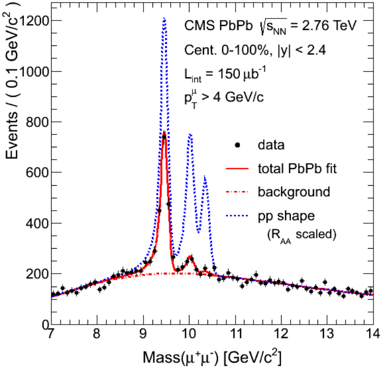
• the number of time-directional lattice sites (N_s) is usually smaller than that of space-directional lattice sites (N_τ) for $T \neq 0$

$\rightarrow$ in other words, we need to obtain more information from lesser amount of temporal correlator lattice data

need to overcome these difficulties somehow.

Quarkonium melting at $T \neq 0$

- does quarkonium exist at $T \neq 0$? If so, at which temperature ?



Quarkonium melting at $T \neq 0$

• potential model consideration: T. Matsui and H. Satz, PLB178 (1986) 416

• first principle calculations ?

- calculate $T \neq 0$ potential between heavy quarks, and solve Schrödinger equation
- calculate relativistic heavy quark correlator and quarkonium spectral functions
- calculate non-relativistic QCD correlator and quarkonium spectral functions

Quarkonium melting at $T \neq 0$

- FASTSUM collaboration:
  - 1st Generation configurations, S- and P-wave correlators: G. Aarts ... SK et al, PRL106 (2011) 277
  - 1st Generation configurations, S-wave: G. Aarts ... SK et al, JHEP1111 (2011) 103
  - 1st Generation configurations, moving S-wave: G. Aarts ... SK et al, JHEP1303 (2013) 084
  - 1st Generation configurations, P-wave: G. Aarts ... SK et al, JHEP1302 (2013) 064
  - 2nd Generation configurations: G. Aarts ... SK et al, JHEP1407 (2014) 097
- KPR:
  - SK A. Rothkopf, P. Petreczky, PRD91 (2015) 054511
  - SK A. Rothkopf, P. Petreczky, JHEP1811(2018) 088)

NRQCD for $T \neq 0$ quarkonium

- m_Q is "integrated out" and focus on the scale of "binding" $\rightarrow$ avoid large scale separation problem
- small statistical errors ($\sim \mathcal{O}(10^{-4})$)
- kernel $K(\tau, \omega)$ becomes $\sim e^{-\omega\tau} \rightarrow$ temperature independent kernel
- intial value problem $\rightarrow$ larger τ range
- continuum limit can't be taken ($m_Q a \sim \mathcal{O}(1)$)

Bayesian methods

- given $G(\tau)$ which is calculated on lattice, what is the spectral function, $\rho(\omega)$?

- Bayes theorm

$$P[X|Y] = P[Y|X]P[X]/P[Y]$$

- in other words

$$P[\rho|D,H] \propto P[D|\rho,H]P[\rho|H]$$

- systematic inclusion of prior knowledge (H)

$$P[D|\rho,H] = e^{-L}, \quad L = \frac{1}{2}\sum_i (D_i - D_i^{\rho})^2/\sigma_i^2$$

and

$$P[\rho|H] = e^{-S}, \quad S = S[\rho(\omega), m(\omega)]$$

where S is the prior and $m(\omega)$ is default model

Bayesian methods

• Shannon-Jaynes entropy for S (cf. Asakwa, Hatsuda, Nakahara, Prog. Part.Nucl.Phys. 45 (2001) 459)

$$S_{SJ} = \alpha \int d\omega \left(\rho - m - \rho \log(\frac{\rho}{m}) \right)$$

• new prior (cf. Y.Burnier, A. Rothkopf, PRL111 (2013) 182003)

$$S_{BR} = \alpha \int d\omega \left(1 - \frac{\rho}{m} + \log(\frac{\rho}{m}) \right)$$

Quarkonium – FASTSUM: NRQCD + MEM

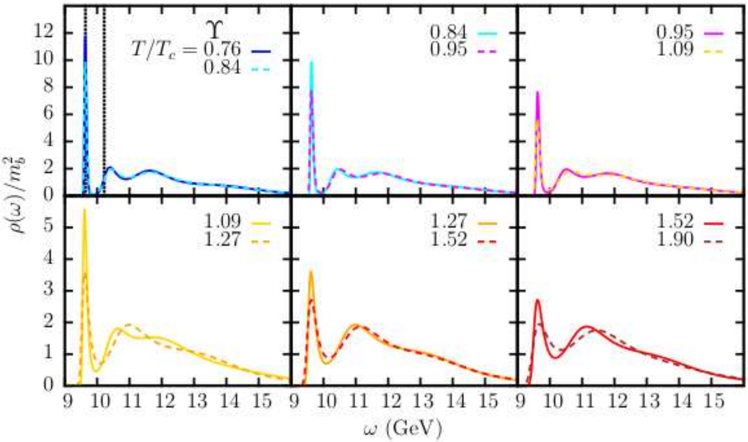
• G. Aarts, C. Allton, T. Harris, S.K., M.P. Lombardo, M.B. Oktay, S.M. Ryan, D.K. Sinclair, J-I. Skullerud: NRQCD + MEM

• anisotropic lattices with fixed scale, T change by N_τ: 1st Gen ($12^3 \times N_\tau, a_s/a_\tau = 6.0, N_f = 2$), 2nd Gen ($24^3 \times N_\tau, a_s/a_\tau = 3.5, N_f = 2+1$), 3rd Gen ($32^3 \times N_\tau, a_s/a_\tau \sim 7, N_f = 2+1$)

• detailed systematic errors study (default-model dependence, energy window, number of configurations, euclidean time window)

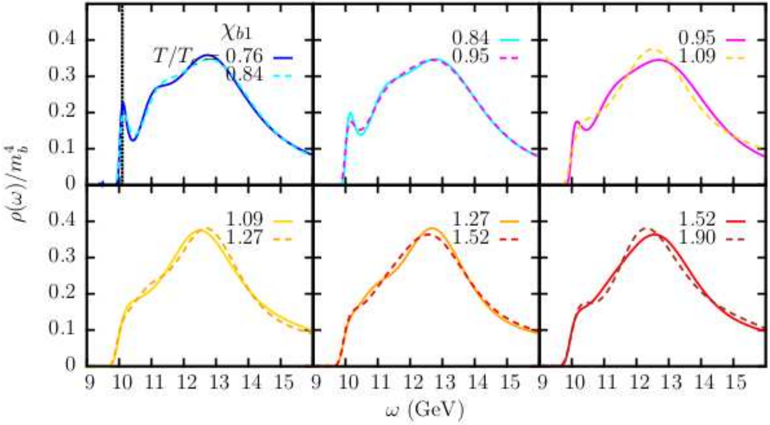
Quarkonium – FASTSUM: NRQCD + MEM

- S-wave (JHEP07 (2014) 097)



Quarkonium – FASTSUM: NRQCD + MEM

- P-wave (JHEP07 (2014) 097)



Quarkonium – FASTSUM: NRQCD + MEM

- sequential suppression of S-wave bottomonium
- survival of $\Upsilon(1S)$ upto $\sim 2.1\,T_c$ (1st Gen) and $\sim 1.9T_c$ (2nd Gen)
- immediate melting of P-wave bottomonium above T_c
- qualitatively similar for both $N_f = 2$ and $N_f = 2+1$ configurations

Quarkonium – KPR: NRQCD + MEM or New Bayesian approach

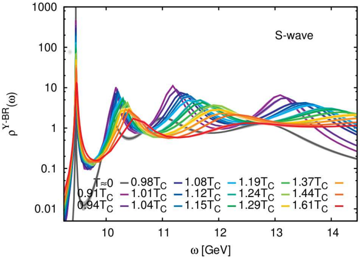
- S.K., A. Rothkopf, P. Petreczky: NRQCD + (MEM, new Bayesian)

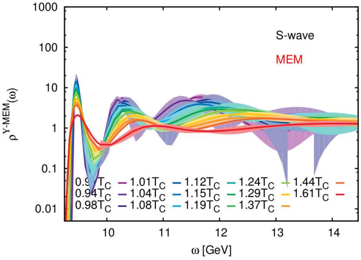
- isotropic lattices from HotQCD ($48^3 \times 12$, $N_f = 2+1$ light $m_\pi \sim 160$ MeV), T change by changing a (needs accompanying $T = 0$ calculation)

- detailed systematic errors study (default-model dependence, energy window, number of configurations, euclidean time window)

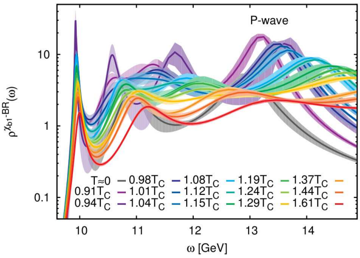
- investigation on the prior dependence (MEM vs new Bayesian)

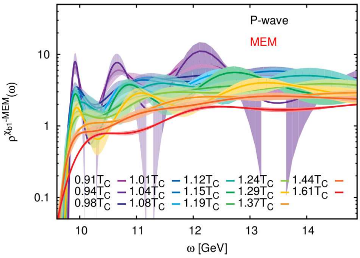
Quarkonium – KPR: NRQCD + MEM or New Bayesian approach





Quarkonium – KPR: NRQCD + MEM or New Bayesian approach

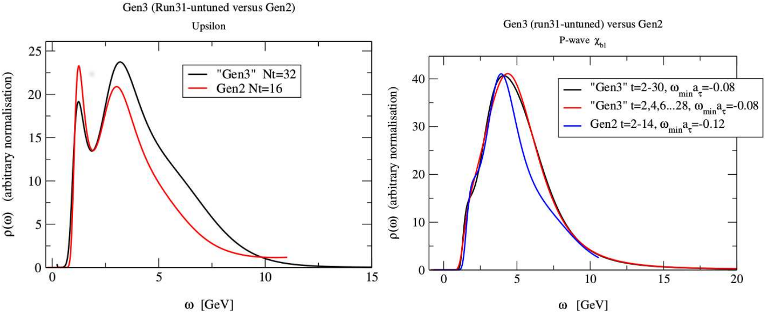




Quarkonium – KPR: NRQCD + MEM or New Bayesian approach

- sequential suppression of S-wave bottomonium
- survival of $\Upsilon(1S)$ upto $\sim 1.6T_c$
- survival of P-wave bottomonium upto $\sim 1.6T_c$

Quarkonium – FASTSUM (preliminary)



Thermal Sommerfeld Effect in QGP

- SK and M. Laine, particle number susceptibility, arXiv:1908.07541
- SK and M. Laine, P-wave, PLB 795 (2019) 469
- SK and M. Laine, dark matter, JCAP1701 (2017) 013
- SK and M. Laine, S-wave, JHEP1607 (2016) 143

Thermal Sommerfeld Effect in QGP

• Lee-Weinberg equation (B.W. Lee and S. Weinberg, PRL39 (1977) 165)

$$\partial_t n = -\langle \sigma_{\rm eff} v \rangle (n^2 - n_{eq}^2)$$

• chemical equilibration rate of heavy quark in Quark-Gluon Plasma (QGP)

• relic density of dark matter particle in early universe

• linearizing Lee-Weinberg equation (SK and M. Laine, JHEP 1607 (2016) 143)

$$\langle \sigma_{\rm eff} v \rangle \equiv \frac{\Gamma_{\rm chem}}{2 n_{eq}}$$

Thermal Sommerfeld Effect in QGP

• for QCD, non-perturbative definition for the chemical/kinetic equilibration rate is necessary

• equilibration rate is a real-time quantity

• lattice gauge theory is a method which can calculate non-perturbative quantities using first principles of quantum field theory

• lattice gauge theory is defined on a Euclidean space and has difficulty in calculating real-time quantity

How to calculate: Usual way

- consider Boltzmann equation*

$$\partial_t n \simeq -c(n^2 - n_{eq}^2) = \dot{n}_{\rm loss} + \dot{n}_{\rm gain}$$

with $\dot{n}_{\rm loss} = -cn^2$

- in equilibrium, $n(t) = n_{\rm eq}$ and $\delta\dot{n} \simeq -2cn\delta n$

$$\Gamma_{\rm chem} = \frac{\delta\dot{n}}{n}\Big|_{\rm eq} = -2\frac{\dot{n}_{\rm loss}}{n_{eq}}$$

- then perturbatively

$$\Gamma_{\rm chem} = \frac{2}{2N_c\int_{\mathbf{k}} f_F(E_k)}\int\int(2\pi)^4\delta^4(P_1+P_2-K_1-K_2)f_F(E_{k_1})f_F(E_{k_2}$$

$$\left(\frac{1}{2}\sum|M_1|^2\,[1+f_B(\varepsilon_{p_1})]\,[1+f_B(\varepsilon_{p_2})]+N_f\sum|M_2|^2\,[1-f_F(\varepsilon_{p_1})]\,[1-f_F(\varepsilon_{p_2})]\right)$$

How to calculate: Usual way

- what if there are bound states?
- various thermal effects (Debye screening, Landau damping, and etc)
- what if there are non-perturbative effect
- Boltzmann equation assumes Boltzmann distribution

$\Gamma_{\rm chem}$ as a transport coefficient

• transport coefficients are usually defined as zero frequency, zero momentum limit of spectral functions of various correlators

• for heavy particle correlators, zero frequency spectral peak is quite narrow and is difficult to access

$\Gamma_{\rm chem}$ as a transport coefficient

• chemical equilibration as a transport coefficient (D. Bödeker, M. Laine, JHEP07 (2012) 130, 01 (2013) 037)

• treat the approach to the equilibrium as a Langevin process

$$\delta\dot{n}(t) = -\Gamma_{\rm chem}\delta n(t) + \xi(t)$$

$$\langle\langle\xi(t)\xi(t')\rangle\rangle = \Omega_{\rm chem}\delta(t-t'), \qquad \langle\langle\xi(t)\rangle\rangle = 0$$

where $\delta n(t)$ is the deviation from the equilibrium and $\xi(t)$ is a stochastic noise

$\Gamma_{\rm chem}$ as a transport coefficient

• to access $\Omega_{\rm chem}$, consider correlators (for heavy quark, or non-relativistic QCD, the heavy quark number is replaced by hamiltonian) in imaginary time

$$\Omega(\tau) = \frac{1}{V}\langle \partial_t H(\tau)\partial_t H(0)\rangle_{\rm qm}$$

or

$$\Delta(\tau) = \frac{1}{V}\langle H(\tau)H(0)\rangle_{\rm qm}$$

then

$$\Omega_{\rm chem} = \lim_{\Gamma_{\rm chem}\ll\omega\ll\omega_{UV}} 2T\frac{\rho_\Omega(\omega)}{\omega} \quad \text{or} \quad = \lim_{\omega\ll T} 2T\omega\rho_\Delta(\omega)$$

and

$$\Gamma_{\rm chem} = \frac{\lim_{\omega\to 0^+} 2T\frac{\rho_\Omega(\omega)}{\omega}}{2\chi_f M^2} \quad \text{or} \quad = \frac{\lim_{\omega\ll T} 2T\omega\rho_\Delta(\omega)}{2\chi_f M^2}$$

$\Gamma_{\rm chem}$ as a transport coefficient

- consider

$$\int_{\vec{x},\vec{y}} \langle H(\tau,\vec{x})\, H(0,\vec{y})\, (\psi^\dagger\chi)(\tau_1,\vec{0})\, (\chi^\dagger\psi)(\tau_2,\vec{0})\rangle\big|_{\tau_1>\tau_2} \left[\theta(\tau-\tau_1)+\theta(\tau_2-\tau)\right]$$

$$= \frac{1}{\mathcal{Z}}\,\mathrm{Tr}\left[e^{-\beta\hat{\mathcal{H}}}(\hat{\psi}^\dagger\hat{\chi})(\tau_1,\vec{0})\,(\hat{\chi}^\dagger\hat{\psi})(\tau_2,\vec{0})\int_{\vec{x},\vec{y}}\hat{H}(0,\vec{x})\hat{H}(0,\vec{y})\right]$$

$$= \frac{1}{\mathcal{Z}}\sum_{m,n}\langle q\bar{q},m|e^{-\beta\hat{\mathcal{H}}}(\hat{\psi}^\dagger\hat{\chi})(\tau_1,\vec{0})\,|n\rangle\,\langle n|(\hat{\chi}^\dagger\hat{\psi})(\tau_2,\vec{0})\int_{\vec{x},\vec{y}}\hat{H}(0,\vec{x})\hat{H}(0,\vec{y})|$$

$$= \frac{4M^2}{\mathcal{Z}}\sum_{m,n} e^{-\beta E_m} e^{(\tau_1-\tau_2)(E_m-\varepsilon_n)}\,\langle q\bar{q},m|\hat{\psi}^\dagger\hat{\chi}|n\rangle\langle n|\hat{\chi}^\dagger\hat{\psi}|q\bar{q},m\rangle$$

E_m are the states with heavy quarks, ε_n are states without heavy quarks

$\Gamma_{\rm chem}$ as a transport coefficient

- with $\mathcal{C}_{mn} = \frac{4M^2}{\mathcal{Z}} e^{-\beta E_m} \langle q\bar{q}, m | \hat{\psi}^\dagger \hat{\chi} | n \rangle \langle n | \hat{\chi}^\dagger \hat{\psi} | q\bar{q}, m \rangle$

$$\varepsilon(\tau) = \sum_{m,n} \mathcal{C}_{mn} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \frac{e^{(\tau_1 - \tau_2)(E_m - \varepsilon_m)}}{\tau_1 - \tau_2} \left[\theta(\tau - \tau_1) + \theta(\tau_2 - \tau)\right]$$

- then with $\omega, \varepsilon_m << E_m$

$$\rho_\Delta(\omega) = \frac{\mathrm{Im} f_1(^1S_0)}{M^2} \sum_{m,n} \mathcal{C}_{mn} \frac{e^{\beta\omega} - e^{-\beta\omega}}{\omega^2}$$

$\Gamma_{\rm chem}$ as a transport coefficient

- finally,

$$
\begin{aligned}
\Omega_{\rm chem} &= \frac{4{\rm Im} f_1({}^1S_0)}{M^2}\sum_{m,n}\mathcal{C}_{mn} \\
&= 16\,{\rm Im} f_1({}^1S_0)\,\frac{1}{\mathcal{Z}}\sum_{m,n} e^{-\beta E_m}\,\langle q\bar{q},m|\hat{\psi}^\dagger\hat{\chi}|n\rangle\langle n|\hat{\chi}^\dagger\hat{\psi}|q\bar{q},m\rangle \\
&= 16\,{\rm Im} f_1({}^1S_0)\,\frac{1}{\mathcal{Z}}\,{\rm Tr}\Big[e^{-\beta\hat{\mathcal{H}}}(\hat{\psi}^\dagger\hat{\chi})(0^+,\vec{0})\,(\hat{\chi}^\dagger\hat{\psi})(0,\vec{0})\Big] \\
&= 16\,{\rm Im} f_1({}^1S_0)\,\Big\langle(\psi^\dagger\chi)(0^+,\vec{0})\,(\chi^\dagger\psi)(0,\vec{0})\Big\rangle
\end{aligned}
$$

$\Gamma_{\rm chem}$ as a transport coefficient

$$P_1 \equiv \frac{1}{2N_c}\mathrm{Re}\left\langle G^{\theta}_{\alpha\alpha;ii}(\beta,\vec{0};0,\vec{0})\right\rangle ,$$

$$P_2 \equiv \frac{1}{2N_c}\left\langle G^{\theta}_{\alpha\gamma;ij}(\beta,\vec{0};0,\vec{0})G^{\theta\dagger}_{\gamma\alpha;ji}(\beta,\vec{0};0,\vec{0})\right\rangle ,$$

$$P_3 \equiv \frac{1}{2N_c^2}\left\langle G^{\theta}_{\alpha\alpha;ij}(\beta,\vec{0};0,\vec{0})G^{\theta\dagger}_{\gamma\gamma;ji}(\beta,\vec{0};0,\vec{0})\right\rangle .$$

- singlet Sommerefeld factor

$$\bar{S}_1 = \frac{P_2}{P_1^2} .$$

- octet Sommerefeld factor

$$\bar{S}_8 = \frac{N_c^2 P_3 - P_2}{(N_c^2-1)P_1^2} .$$

$\Gamma_{\rm chem}$ as a transport coefficient

• P-wave Sommerfeld factor

$$\bar{S}_p = \frac{P_p}{M^2 P_1^2}$$

with

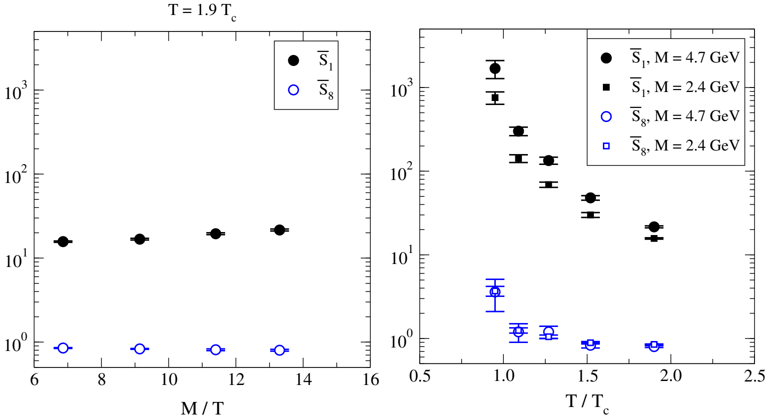
$$p_p = \mathrm{Tr}\langle \Delta_i G_V(\beta,\vec{0};0,\vec{0};i) G^\dagger(\beta,\vec{0};0,\vec{0})\rangle - \mathrm{Tr}\langle G_V(\beta,\vec{0};0,\vec{0};i)\Delta_i G^\dagger(\beta,\vec{0};0,\vec{0})\rangle$$

• P-wave state may have a better signal-to-noise ratio in an experimental situation or a better detection strategy

• bound states are important in thermal Sommerfeld effect and P-wave has lower melting temperature

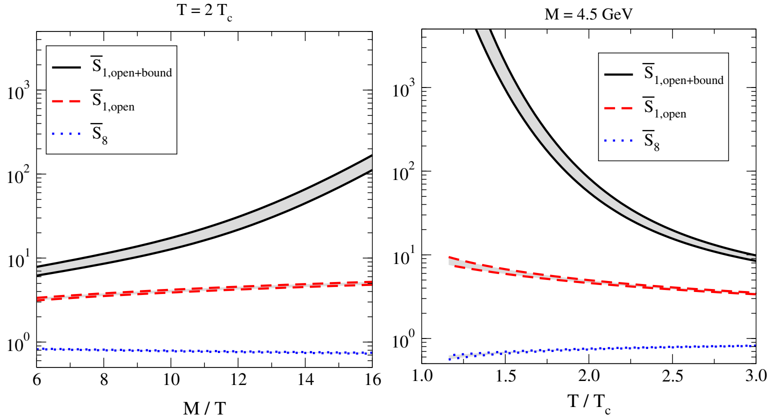
Lattice result of thermal Sommerfeld factor (S-Wave)

- SK and M. Laine, JHEP1607 (2016) 143

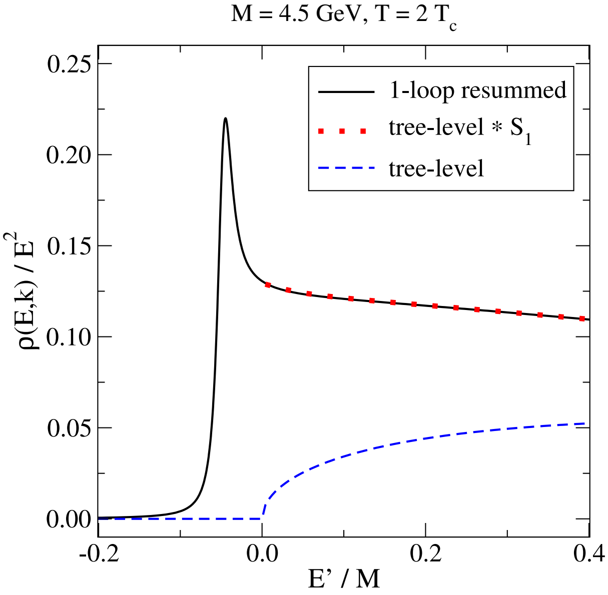


Analytic estimate of thermal Sommerfeld factor (S-wave)

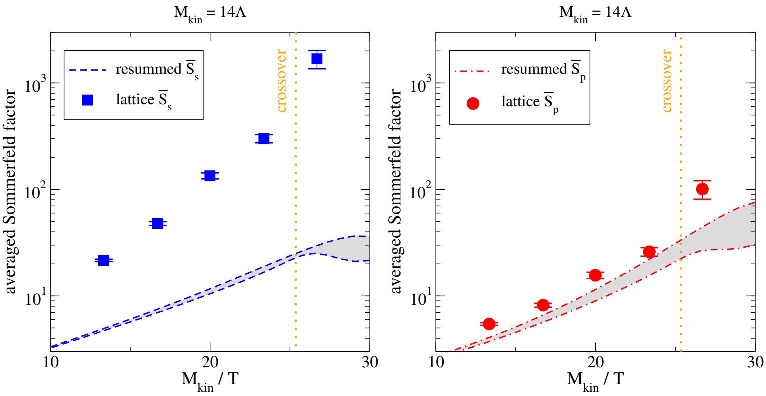
- SK and M. Laine, JHEP1607 (2016) 143



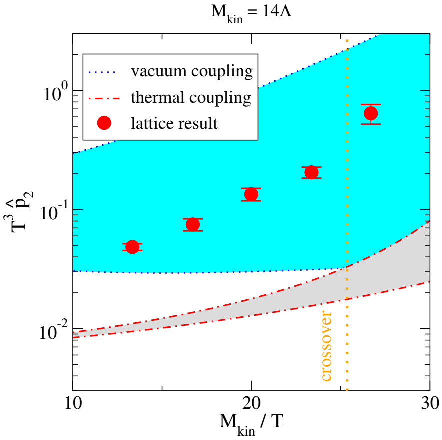
Analytic estimate of thermal Sommerfeld factor (S-wave)



Lattice result of thermal Sommerfeld factor (S & P-Wave)



Non-relativistic particle susceptibility



Discussion

• Many interesting quantities related to quarkonium at $T \neq 0$ can be calculated using lattice NRQCD

• The main problem which affects a systematic computation of quarkonium spectral function at $T \neq 0$ becomes less troublesome

• Lattice NRQCD + Bayesian method may give us quantitative answer to in-medium modification of quarkonium spectral function

• For the first time, a real time quantity related to heavy quark chemical equilibration is calculated using lattice NRQCD

• The number density of heavy dark matter (interacting under non-perturbative, non-abelian gauge theory) in early universe may be understood using lattice NRQCD