

Y. Sumino (Tohoku Univ.)

Plan of talk

- 1. Technical developments
- 2. Physics predictions
- 3. Challenge (Analytic evaluation of a_3)
- 4. Summary

Heavy quarkonium states $(t\bar{t}, b\bar{b}, c\bar{c}, b\bar{c})$

Unique system: Properties of individual hadrons predictable in pert. QCD

Two theoretical foundations for computing higher-order corr. systematically

- Threshold expansion
- EFT (pNRQCD, vNRQCD)

Beneke, Smirnov

Pineda, Soto, Brambilla, Vairo Luke, Manohar, Rothstein Computation of quarkonium spectrum up to NNNLO

Kiyo, YS: 1408.5590

$$\mathcal{L}_{\text{pNRQCD}} = S^{\dagger} (i\partial_t - \widehat{H}_S)S + O^{a\dagger} (iD_t - \widehat{H}_O)^{ab}O^b + g S^{\dagger} \vec{r} \cdot \vec{E}^a O^a + \cdots$$

Energy levels given by poles of the full propagator of S in pNRQCD.



e.g.
$$A(n, \ell) = \sum_{k=1}^{\infty} \frac{(n-\ell+k-1)!}{(n+\ell+k)!k^3}$$

$$\frac{(n-\ell+k-1)!}{(n+\ell+k)!} = \prod_{m=-\ell}^{\ell} \frac{1}{n+k+m} = \sum_{m=-\ell}^{\ell} \frac{R(\ell,m)}{n+k+m}, \qquad R(\ell,m) = \frac{(-1)^{\ell-m}}{(\ell+m)!(\ell-m)!}$$

$$\sum_{k=1}^{\infty} \frac{1}{(k+i)k^3} = \frac{\zeta(3)}{i} - \frac{\zeta(2)}{i^2} + \frac{S_1(i)}{i^3} \quad \text{where } S_1(i) = \sum_{k=1}^{i} \frac{1}{k} \text{ denotes the harmonic sum.}$$

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A general algorithm exists, Anzai, YS which can evaluate, e.g.

$$f(i) = \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^{m-k}}{(k+i)^2 (k+m+i) (m+2i+1)}$$

 $i \to i + \Delta i, \quad k \to k + \Delta k,$ $m \to m + \Delta m$

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$$f(i) = \sum_{k=1}^{\infty} \sum_{m=1}^{\infty} \frac{(-1)^{m-k}}{(k+i)^2 (k+m+i)(m+2i+1)}$$

Reduced to a combination of nested sums:

$$Z(i; \{b_j\}; \{\lambda_j\}) = \sum_{i \ge n_1 > n_2 > \dots > n_N > 0} \frac{\lambda_1^{n_1} \lambda_2^{n_2} \cdots \lambda_N^{n_N}}{n_1^{b_1} n_2^{b_2} \cdots n_N^{b_N}}$$

$$i \to i + \Delta i, \quad k \to k + \Delta k, m \to m + \Delta m$$

 $(b_j \in \mathbb{N}, \lambda_j \in \text{roots of unity})$

Algebraic derivation of US correction (QCD Bethe log)

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Brambilla, Pineda, Soto, Vairo Kniehl, Penin

$$\begin{split} E_{n\ell}^{\rm us} &= -ig^2 \bar{\mu}^{2\epsilon} \frac{T_F}{N_C} \int_0^\infty dt \langle \vec{r} \cdot \vec{E}^a(t,\vec{0}) \exp\left[-i\left(H_O^{(d)} - E_{n,C}^{(d)}\right)t\right] \vec{r} \cdot \vec{E}^a(0,\vec{0}) \rangle_{n\ell} \\ &= \frac{1}{2} C_F g^2 \bar{\mu}^{2\epsilon} \frac{1-d}{d} C(d) \langle r^i \left(H_O^{(d)} - E_{n,C}^{(d)}\right)^d r^i \rangle_{n\ell}. \qquad d = D - 1 = 3 - 2\epsilon \end{split}$$

$$\left\langle E^{ia}(t,\vec{0})E^{ja}(0,\vec{0})\right\rangle = -i\delta^{aa}\int \frac{d^Dk}{(2\pi)^D} \frac{e^{ik_0t}}{k^2 + i0} \left(k^ik^j - k_0^2\delta^{ij}\right) + \mathcal{O}(\alpha_s)$$



Brambilla, Pineda, Soto, Vairo Kniehl, Penin

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up to $O(\epsilon)$ necessary $(H_{O}^{(d)} - E_{n,C}^{(d)})^{3-2\epsilon} \approx (H_{O}^{(d)} - E_{n,C}^{(d)})^{3} [1 - 2\epsilon \log(H_{O}^{(d)} - E_{n,C}^{(d)})]$ $\bar{\mu}^{2\epsilon} \langle r^{i} (H_{O}^{(d)} - E_{n,C}^{(d)})^{d} r^{i} \rangle_{n\ell} = \langle X - 2\epsilon r^{i} (H_{O}^{(3)} - E_{n,C}^{(3)})^{3} \log \left(\frac{H_{O}^{(3)} - E_{n,C}^{(3)}}{\bar{\mu}}\right) r^{i} \rangle_{n\ell} + \mathcal{O}(\epsilon^{2})$ $X = r^{i} (H_{O}^{(d)})^{3} r^{i} - \frac{3}{2} \{ H_{S}^{(d)}, r^{i} (H_{O}^{(d)})^{2} r^{i} \} + \frac{3}{2} \{ (H_{S}^{(d)})^{2}, r^{i} H_{O}^{(d)} r^{i} \} - \frac{1}{2} \{ (H_{S}^{(d)})^{3}, \bar{r}^{2} \}$

Use commutation relation $[r_i, p_j] = i \delta_{ij}$ and $\langle n | [H_S, \sigma] | n \rangle = 0$ to simplify *X*.



Brambilla, Pineda, Soto, Vairo Kniehl, Penin

$$\begin{split} E_{n\ell}^{\mathrm{us}} &= -ig^{2}\bar{\mu}^{2\epsilon}\frac{T_{F}}{N_{C}}\int_{0}^{\infty}dt \langle \vec{r}\cdot\vec{E}^{a}(t,\vec{0})\exp\left[-i\left(H_{O}^{(d)}-E_{n,C}^{(d)}\right)t\right]\vec{r}\cdot\vec{E}^{a}(0,\vec{0})\rangle_{n\ell} \\ &= \frac{1}{2}C_{F}g^{2}\bar{\mu}^{2\epsilon}\frac{1-d}{d}C(d) \langle r^{i}\left(H_{O}^{(d)}-E_{n,C}^{(d)}\right)^{d}r^{i}\rangle_{n\ell}, \qquad d=D-1=3-2\epsilon \\ &= \langle H^{\mathrm{us}}\rangle_{n\ell} - \frac{2C_{F}\alpha_{s}}{3\pi} \langle r^{i}\left(H_{O}^{(3)}-E_{n,C}^{(3)}\right)^{3}\log\left(\frac{H_{O}^{(3)}-E_{n,C}^{(3)}}{\mu}\right)r^{i}\rangle_{n\ell}. \end{split}$$



• Scale dependence



Use MS mass Marquard, Smirnov, Smirnov, Steinhauser • $\overline{m}_b, \overline{m}_c$ determination

Kiyo, Mishima, YS



PDG value $\overline{m}_c = 1275 \pm 25$ MeV

 $\overline{m}_{b}^{\text{ave}} = 4197 \pm 2 \ (d_3) \ \pm 6 \ (\alpha_s) \ \pm 20 \ (\text{h.o.}) \pm 5 \ (m_c) \ \text{MeV}$

PDG value $\overline{m}_b = 4.18 \pm 0.03 \text{ GeV}$



<u>3. Challenge</u>: Analytic evaluation of a_3 (3-loop QCD potential)



 $= \sum_{k} r_{k} Z\left(\infty; \{b_{i}^{(k)}\}; \{\lambda_{i}^{(k)}\}\right) + C_{0}$ Generalized MZVs $Z(\infty; \{b_i\}; \{\lambda_i\}) = \sum_{\substack{n_1 > n_2 > \dots > n_N > 0}} \frac{\lambda_1^{n_1} \lambda_2^{n_2} \cdots \lambda_N^{n_N}}{n_1^{b_1} n_2^{b_2} \cdots n_N^{b_N}} \qquad (b_i \in \mathbb{N}, \ \lambda_i \in \mathbb{C})$

Unknown expansion coefficient in ϵ

Not reducible to MZVs (as yet)

Colleagues are invited to reveal the nature of this extension(?) of MZVs.

<u>Summary</u>

- Non-relativistic bound-state theory for QED/QCD has become fairly mature and amenable to a textbook-level understanding and computations.
- Recently NNNLO corrections to the <u>complete spectrum</u> and <u>Kiyo, YS</u> threshold production cross section have been computed. <u>Beneke, Kiyo, Marquard, Penin, Piclum, Steinhauser</u>

Applied a new technology for evaluating multiple sums; All computations arithmetic (no diagrammatic analysis).

Challenge: Analytic evaluation of a_3 remains

• Applications

Bottomonium spectroscopy at NNNLO: reasonable agreement with exp. data. Kiyo, YS \overline{m}_b and $\overline{m}_c \overline{\text{MS}}$ mass determination from $J/\psi(1S)$, $\eta_c(1S)$ and $\Upsilon(1S)$, $\eta_b(1S)$.

Kiyo, Mishima, YS:



Postdictions or predictions?

- Fine and hyperfine splittings of charmonium/bottomonium reproduced.
 - Two exceptions around 2003:Recksiegel, Y.S.;Kniehl, Penin,charmonium hyperfine splitting $\Psi(2S) \eta_c(2S)$ Pineda, Smirnov, Steinhauserbottomonium hyperfine splitting $\Upsilon(1S) \eta_b(1S)$ Both are solved in favor of pert.QCD predictions.

Slides from Skwarnicki's plenary talk at Lepton-Photon 2003



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b-QUARK MS MASS (GeV)

e.g.
$$A(n, \ell) = \sum_{k=1}^{\infty} \frac{(n-\ell+k-1)!}{(n+\ell+k)!k^3}$$

$$\frac{(n-\ell+k-1)!}{(n+\ell+k)!} = \prod_{m=-\ell}^{\ell} \frac{1}{n+k+m} = \sum_{m=-\ell}^{\ell} \frac{R(\ell,m)}{n+k+m}, \qquad R(\ell,m) = \frac{(-1)^{\ell-m}}{(\ell+m)!(\ell-m)!}$$

$$\sum_{k=1}^{\infty} \frac{1}{(k+i)k^3} = \frac{\zeta(3)}{i} - \frac{\zeta(2)}{i^2} + \frac{S_1(i)}{i^3} \quad \text{where } S_1(i) = \sum_{k=1}^{i} \frac{1}{k} \text{ denotes the harmonic sum.}$$

$$= \sum_{k=1}^{\infty} \left[\frac{1}{i} \frac{1}{k^3} - \frac{1}{i^2} \frac{1}{k^2} + \frac{1}{i^3} \left(\frac{1}{k} - \frac{1}{k+i} \right) \right]$$

$$= \frac{1}{i} \zeta(3) - \frac{1}{i^2} \zeta(2) + \frac{1}{i^3} \sum_{k=1}^{\infty} \left(\frac{1}{k} - \frac{1}{k+i} \right)$$

$$\frac{1}{k} + \frac{1}{k+1} + \dots + \frac{1}{i} \equiv S_1(i)$$

$$f(m) = \sum_{k=1}^{\infty} \frac{(-1)^k}{(1+k+m)^2}.$$
(20)

This can be expressed as

$$f(m) = [f(m) + f(m-1)] - [f(m-1) + f(m-2)] + \dots + (-1)^{m} [f(2) + f(1)] - (-1)^{m} f(1) = \sum_{j=2}^{m} (-1)^{m-j} [f(j) + f(j-1)] - (-1)^{m} f(1).$$
(21)

Bulk of the sum in the "difference" of two adjacent terms gets canceled since the shifts $m \rightarrow m-1$, $k \rightarrow k + 1$ leave the denominator in Eq. (20) unchanged

$$f(j) + f(j-1) = \left(\sum_{k=1}^{\infty} -\sum_{k=2}^{\infty}\right) \frac{(-1)^k}{(k+j)^2} = \frac{-1}{(j+1)^2}.$$
 (22)

Thus,

$$f(m) = (-1)^m \sum_{j=2}^m \frac{(-1)^{1-j}}{(j+1)^2} - (-1)^m \sum_{k=1}^\infty \frac{(-1)^k}{(k+2)^2}.$$
(23)

In the first term, apart from the coefficient $(-1)^m$, dependence on the external index *m* enters only through the upper bound of the summation, while the second term, apart from $(-1)^m$, is free of *m* and is essentially an MZV.

$$\begin{split} H_{S}^{(d)} &= \frac{\hat{\vec{p}}^{2}}{m} + V_{S}^{(d)}(r), \qquad H_{O}^{(d)} = \frac{\hat{\vec{p}}^{2}}{m} + V_{O}^{(d)}(r), \\ V_{S}^{(d)}(r) &= -C_{F} \frac{\alpha_{s}}{r} (\bar{\mu}r)^{2\epsilon} A(\epsilon), \qquad V_{O}^{(d)}(r) = \left(\frac{C_{A}}{2} - C_{F}\right) \frac{\alpha_{s}}{r} (\bar{\mu}r)^{2\epsilon} A(\epsilon), \\ A(\epsilon) &= \frac{\Gamma(\frac{1}{2} - \epsilon)}{\pi^{\frac{1}{2} - \epsilon}}. \end{split}$$

Regularization needed to deal with $\delta(\vec{r})$ in commutation relations.

$$V_S^{(d)}(r) \to -C_F \frac{\alpha_s}{r} (\bar{\mu}r)^{2(\epsilon+u)} A(\epsilon),$$

$$V_O^{(d)}(r) \to \left(\frac{C_A}{2} - C_F\right) \frac{\alpha_s}{r} (\bar{\mu}r)^{2(\epsilon+u)} A(\epsilon).$$

$$X = r^{i} (H_{O}^{(d)})^{3} r^{i} - \frac{3}{2} \{ H_{S}^{(d)}, r^{i} (H_{O}^{(d)})^{2} r^{i} \} + \frac{3}{2} \{ (H_{S}^{(d)})^{2}, r^{i} H_{O}^{(d)} r^{i} \} - \frac{1}{2} \{ (H_{S}^{(d)})^{3}, \vec{r}^{2} \}$$

$$\begin{split} X &= -\frac{4\alpha_s A \, C_A(2u^2 + u(4\epsilon - 1) + \epsilon(2\epsilon - 1))(\bar{\mu}r)^{2(u+\epsilon)}}{m^2 r^3} r^i r^j \, \hat{p}^j \, \hat{p}^i \\ &+ \frac{\alpha_s^3 A^3 C_A^3(\bar{\mu}r)^{6(u+\epsilon)}}{8r} \\ &+ \frac{4\alpha_s A \, u(2u + 2\epsilon - 1)(C_A(u+1)(u+\epsilon) - C_F)(\bar{\mu}r)^{2(u+\epsilon)}}{m^2 r^3} \\ &+ \frac{\alpha_s^2 A^2 C_A[C_A(2u^2 + 4u(\epsilon + 1) + 2\epsilon^2 + \epsilon + 2] - 4C_F(2u^2 + 4u\epsilon + u + 2\epsilon^2 + \epsilon - 1)](\bar{\mu}r)^{4(u+\epsilon)}}{2mr^2} \\ &+ \frac{2\alpha_s A C_A\{8u^3 + 4u^2(4\epsilon + 1) + 2u(4\epsilon^2 + 6\epsilon - 3) + 8\epsilon^2 - 6\epsilon + 1\}(\bar{\mu}r)^{2(u+\epsilon)}}{m^2 r^3} i \vec{r} \cdot \hat{\vec{p}} \\ &- \frac{2\alpha_s A C_A(2u + 2\epsilon - 1)(\bar{\mu}r)^{2(u+\epsilon)}}{m^2 r} \, \hat{p}^2. \end{split}$$

$$\left[H_{S}^{(3)}, \frac{C_{F}\alpha_{s}}{4mr}\left(\frac{1}{2} - i\vec{r}\cdot\hat{\vec{p}}\right)\right] = -\frac{C_{F}\alpha_{s}}{4m^{2}}\left\{\frac{1}{r}, \hat{\vec{p}}^{2}\right\} + \frac{\pi C_{F}\alpha_{s}}{m^{2}}\delta^{3}(\vec{r}) + \frac{C_{F}\alpha_{s}}{2m^{2}r^{3}}r^{i}r^{j}\hat{p}^{j}\hat{p}^{i} + \frac{C_{F}^{2}\alpha_{s}^{2}}{4mr^{2}},$$

Reduction of MZVs with various λ_i s

e.g. $\lambda_i \in \{\pm 1, \pm e^{\pm \pi i/4}, \pm \frac{1 \pm 2i}{\sqrt{5}}, \pm i\}$

Shuffle relations are ineffective for reduction in such cases, too many variables, insufficient constraints,...

We reduced MZVs to a smaller set in the following way. Let $\omega_8 \equiv e^{\pi i/4}$, $Q \equiv \frac{1+2i}{\sqrt{5}}$, and type ω_8 : $\lambda_i = \omega_8^p$ type Q: $\lambda_i = Q^p \omega_8^{p'}$ $p, p' \in \mathbb{Z}$

• Convert MZVs using the algorithm 1 in Anzai's talk:



then use shuffle relations in integral rep.

 $\bullet \ Q \to Q^{-1}, \ Q \to Q^2$

Physics predictions

At NNLO (~2000)

- Global level structure of bottomonium is reproduced.
 Brambilla, Y.S., Vairo
- Fine and hyperfine splittings of charmonium/bottomonium reproduced.
 - Two exceptions in ~2003:Recksiegel, Y.S.;Kniehl, Penin,charmonium hyperfine splitting $\Psi(2S) \eta_c(2S)$ Pineda, Smirnov, Steinhauserbottomonium hyperfine splitting $\Upsilon(1S) \eta_b(1S)$ Solved in favor of pert.QCD predictions.

At NNNLO

$$Z\left(\infty; a_1, a_2, \dots, a_N; \lambda_1, \lambda_2, \dots, \lambda_N\right) = \sum_{\substack{n_1 > n_2 > \dots > n_N > 0}} \frac{\lambda_1^{n_1} \lambda_2^{n_2} \cdots \lambda_N^{n_N}}{n_1^{a_1} n_2^{a_2} \cdots n_N^{a_N}} \quad ; \quad a_i \in \mathbb{N}$$

 $\begin{array}{ll} \lambda_i \in \{1\} & \text{MZV} \\ \lambda_i \in \{-1,1\} & \text{Sign-alternating Euler sum} \\ \lambda_i \in \text{Roots of unity} & \text{e.g. } \lambda_i = e^{i\pi/3} \\ \lambda_i \in \mathbb{C} & \text{generalized MZV} \end{array}$

pNRQCD Lagrangian

 $Q\bar{Q}$ composite fields





 $\begin{aligned} \mathcal{L}_{\text{pNRQCD}} &= S^{\dagger} \big(i \partial_t - \widehat{H}_S \big) S + O^{a \dagger} \big(i D_t - \widehat{H}_O \big)^{ab} O^b \\ &+ g \, S^{\dagger} \vec{r} \cdot \vec{E}^a O^a + g \, O^{a \dagger} \vec{r} \cdot \vec{E}^a S + \cdots \end{aligned}$

Color electric field $\vec{E}^a = -\vec{\nabla}A_0^a - \partial_t \vec{A}^a - gf^{abc}A_0^b \vec{A}^c$ at position \vec{X} , originating from multipole exp. of $A_\mu(\vec{X} \pm \vec{r}/2)$ in \vec{r} .

 \hat{H}_{S} , \hat{H}_{O} : Quantum mechanical Hamiltonian for singlet and octet states

$$\left(\widehat{H}_{S}\right)_{LO} = \frac{\overrightarrow{p}^{2}}{m} - C_{F} \frac{\alpha_{S}}{r}, \qquad \left(\widehat{H}_{O}\right)_{LO} = \frac{\overrightarrow{p}^{2}}{m} + \left(\frac{C_{A}}{2} - C_{F}\right) \frac{\alpha_{S}}{r}$$

$$\implies \beta \sim \frac{p}{m} \sim \frac{1}{mr} \sim \alpha_{S} \qquad \text{(in the c.m. frame)}$$

$$\begin{split} \left(\hat{H}_{S}\right)_{LO} &= \frac{\vec{p}^{2}}{m} - C_{F} \frac{\alpha_{s}}{r}, \\ \left(\hat{H}_{S}\right)_{NLO} &= -C_{F} \frac{\alpha_{s}}{r} \cdot \left(\frac{\alpha_{s}}{4\pi}\right) \cdot \{\beta_{0} \log\left(\mu'^{2}r^{2}\right) + a_{1}\}, \\ \left(\hat{H}_{S}\right)_{NNLO} &= -\frac{\vec{p}^{4}}{4m^{3}} - C_{F} \frac{\alpha_{s}}{r} \cdot \left(\frac{\alpha_{s}}{4\pi}\right)^{2} \cdot \left\{\beta_{0}^{2} \left[\log^{2}\left(\mu'^{2}r^{2}\right) + \frac{\pi^{2}}{3}\right] + \left(\beta_{1} + 2\beta_{0}a_{1}\right) \log\left(\mu'^{2}r^{2}\right) + a_{2}\right\} \\ &+ \frac{\pi C_{F} \alpha_{s}}{m^{2}} \delta^{3}(\vec{r}) + \frac{3C_{F} \alpha_{s}}{2m^{2}r^{3}} \vec{L} \cdot \vec{S} - \frac{C_{F} \alpha_{s}}{2m^{2}r} \left(\vec{p}^{2} + \frac{1}{r^{2}}r_{i}r_{j}p_{j}p_{i}\right) - \frac{C_{A} C_{F} \alpha_{s}^{2}}{2mr^{2}} \\ &- \frac{C_{F} \alpha_{s}}{2m^{2}} \left\{\frac{\vec{S}^{2}}{r^{3}} - 3\frac{\left(\vec{S} \cdot \vec{r}\right)^{2}}{r^{5}} - \frac{4\pi}{3}\left(2\vec{S}^{2} - 3\right)\delta^{3}(\vec{r})\right\} \end{split}$$

 $(\widehat{H}_S)_{NNNLO}$ = known (Wilson coeffs. include IR div.)

Kniehl, Penin, Smirnov, Steinhauser (a_3 : Anzai, Kiyo, YS; Smirnov, Steinhauser)

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At NNNLO

