Inverse Monte Carlo Methods

Wozar, Kaestner, Wipf and Heinz , PRD 76 (2007)

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Outline

- Effective models for Yang-Mills theory
- Algebraic and geometric Schwinger-Dyson equations
- Inverse Monte Carlo **SU(2) case: Gonzalez-Arroyo and Okawa PRD (1987), Deckert, Wansleben, Zabolitzky PRD (1987)**
- Results for SU(3) Yang-Mills theory

Center Symmetry and Deconfinement

- Deconfinement trans for YM second-order for SU(2) and first-order for SU(3) in (3+1)
  - Wilson line is the order parameter $P(x) = tr\left(\mathcal{T} e^{ig\int_0^\beta d\tau A_0(\tau,x)}\right)$
  - Non-periodic gauge transformations: $U_0(\tau+\beta, x) = zU(\tau, x),\ z \in Z_3$
  - YM action invariant while $P \to zP$
  - VEV of P zero in confined phase, nonzero in deconfined phase
  - LG free-energy $F[P]$ by integrating out other degrees of freedom
  - $(d+1)$ YM at $T \neq 0$ described by spin-model in d dimensions

Svetitsky and Yaffe, Nucl. Phys. B (1982)

Effective Action

- Building blocks of action traces of Polyakov loop in a rep. r (characters)

$$\mathscr{P}^{(r)}(\vec{x}) \equiv \prod_{\tau=1}^{N_\tau} U_0^{(r)}(\tau, \vec{x}),\ r \equiv (p,q) \qquad \chi_r(\mathscr{P}) \equiv tr\mathscr{P}_r$$

- Characters of higher-dim. reps only depend on characters of fundamental and antifundamental r

$$\chi_{(1,0)}(\mathscr{P}) = P,\ \chi_{(0,1)}(\mathscr{P}) = P*$$

- Effective action should be invariant under a center transformation

$$\chi_{(p,q)} \to z\chi_{(p,q)},\ z \in Z_3$$

- From strong-coupling expansions, we know that to leading order we should have NN couplings

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Effective Action

- General form of action consistent with center symmetry (NN only)

$$S_{eff}^{(NN)}[\chi] = \sum_{<x,y>} \sum_{p,q,p',q'} \delta_{p+p',q+q'+3\tilde{n}} \, \lambda_{p,q,p',q'} \chi_{pq}(\mathscr{P}_x) \, \chi_{p'q'}(\mathscr{P}_y)$$

- "Local" terms included when (p,q)=(0,0)

- Couplings λ_i unknown!

- Should have β-dependance and should decrease as dim. of reps labeling it increase

$$S_{eff} = \sum_i \lambda_i S_i$$

Where to truncate?

Effective Action

- From strong coupling, we know what terms enter at a given order $O(\beta^{kN_\tau})$

- Rewrite the effective action in a different basis (polymer)

$$S_{eff}[\chi] = \sum_{r} \sum_{\{\mathcal{R}_i\}} \sum_{\{l_i\}} c^{l_1 \ldots l_r}_{\mathcal{R}_1 \ldots \mathcal{R}_r} \prod_{i=1}^{r} S_{\mathcal{R}_i, l_i}$$

$$S_{\mathcal{R},l} \equiv \chi_{\mathcal{R}}(\mathcal{P}_x)\chi^*_{\mathcal{R}}(\mathcal{P}_y) + c.c.$$

 # links **reps** **links** $l_i \equiv \; < x_i, y_i >$

- Conditions on summation: $r \leq k, \; \sum_i (p_i + q_i) < k$

- Lowest order $O(\beta^{N_\tau})$ gives familiar generalized Potts model

$$S^{(0)}_{eff} = \kappa_1 \sum_{<x,y>} \left(\mathcal{P}_x \mathcal{P}^*_y + c.c. \right)$$

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Schwinger-Dyson Equations

- Need to relate effective actions to full Yang-Mills theory (no fermions)

$$0 = < \frac{\delta S_{eff}(\lambda)}{\delta \phi} >_{eff} = < \frac{\delta S_{eff}(\lambda)}{\delta \phi} >_{YM}$$

relationship holds for full effective theory

produce configs. with Y-M action

- Need to relate couplings in effective action to full Yang-Mills theory (no fermions)

- Schwinger-Dyson equations: equations of motion satisfied by correlation function

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Algebraic SDEs

- Parametrize Polyakov loop using angular variables ($\det \mathscr{P} = 1$)

$$\mathscr{P}(\phi_1, \phi_2) = diag(e^{i\phi_1}, e^{i\phi_2}, e^{-i(\phi_1+\phi_2)})$$

- In our effective theory we consider class functions which are constant on each class

$$f(U) = f(VUV^{-1}),\ V \in SU(3)$$

- Class functions constant on each class (integrate over redundant d.o.f.)

$$\int dU_{red} f(U) = \int d\phi_1 d\phi_2 \det\left(\frac{\partial \chi_p}{\partial \phi_j}\right) f(U)$$

$$\boxed{dU_{red} = J^{1/2} dP dP^*} \qquad J(P, P^*) \equiv \det\left(\frac{\partial \chi_p}{\partial \phi_j}\right)$$

- If a class function f vanishes on the boundary of fundamental region $\partial\Omega$

$$\int_\Omega dP dP^* \partial_P f = 0$$

"integration by parts"

Choice: $J^{3/2} \dfrac{\partial h}{\partial P_x^*} e^{-S_{eff}}$

Boltzmann weight!

Algebraic SDEs

- Functions h need to be center-symmetric!

$$h(P, P^*) = h(zP, z^*P^*)$$

- Attach site labels x, z which range over the entire lattice

$$0 = \int dU_{red} \left(\frac{3}{2} \frac{\partial J_z}{\partial P_z} \frac{\partial h}{\partial P_x^*} e^{-S_{eff}} + J \frac{\partial}{\partial P_z} \left(\frac{\partial h}{\partial P_x^*} e^{-S_{eff}} \right) \right)$$

- Derivative of effective action brings down terms linear in λ_i

$$0 = < \frac{3}{2} \frac{\partial J_z}{\partial P_z} \frac{\partial h}{\partial P_x^*} + J_z \frac{\partial^2}{\partial P_x^* \partial P_z} > - \sum_i \lambda_i < J \frac{\partial h}{\partial P_x^*} \frac{\partial S_i}{\partial P_z} >$$

expectation value wrt YM action

- Choose h from among the terms S_i

Geometric SDEs

Uhlmann, Mienel, Wipf, JPhysA 40 (2007)

- Alternate formulation which gives set of equations involving λ_i
- Start from invariance of the Haar measure: $\int dU\ L_a f(U) = 0 \quad L_a f(U) \equiv \frac{d}{dt} f(e^{tT_a}U)\,|_{t=0}$
- Want $L_a f$ to be a class function: $f = g\ L_a \chi_r$, where g is a class function
- Can now integrate over reduced Haar measure!
- Can express left Lie derivatives in terms of EV of quadratic Casimir op. and CG coefficients

$$L_a L^a \chi_r = -\,c_p \chi_r \qquad L_a \chi_r L^a \chi_{r'} = \frac{1}{2}\left[(c_r + c_{r'})\chi_r \chi_{r'} - \sum_\rho C^\rho_{r,r'} c_\rho \chi_\rho \right]$$

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Geometric SDEs

- Again, appropriate choice for class function: $g = \dfrac{\partial S_i}{\partial P_x} e^{-S_{eff}}$

- Convert into separate set of coupled equation

$$\boxed{\begin{aligned} 0 = \langle -\frac{16}{3} P_z \frac{\partial S_i}{\partial P_x} + \left(r P_z^* - 4/3 P_z^2\right) \frac{\partial^2 S_i}{\partial P_x \partial P_z} + \left(6 - 2/3 |P_z|^2\right) \frac{\partial^2 S_i}{\partial P_x \partial P_z^*} \rangle \\ - \sum_j \lambda_j \langle \left(4 P_z^* - 4/3 P_z^2\right) \frac{\partial S_i}{\partial P_x} \frac{\partial S_j}{\partial P_z} + \left(6 - 2/3 |P_z|^2\right) \frac{\partial S_i}{\partial P_x} \frac{\partial S_j}{\partial P_z^*} \rangle \end{aligned}}$$

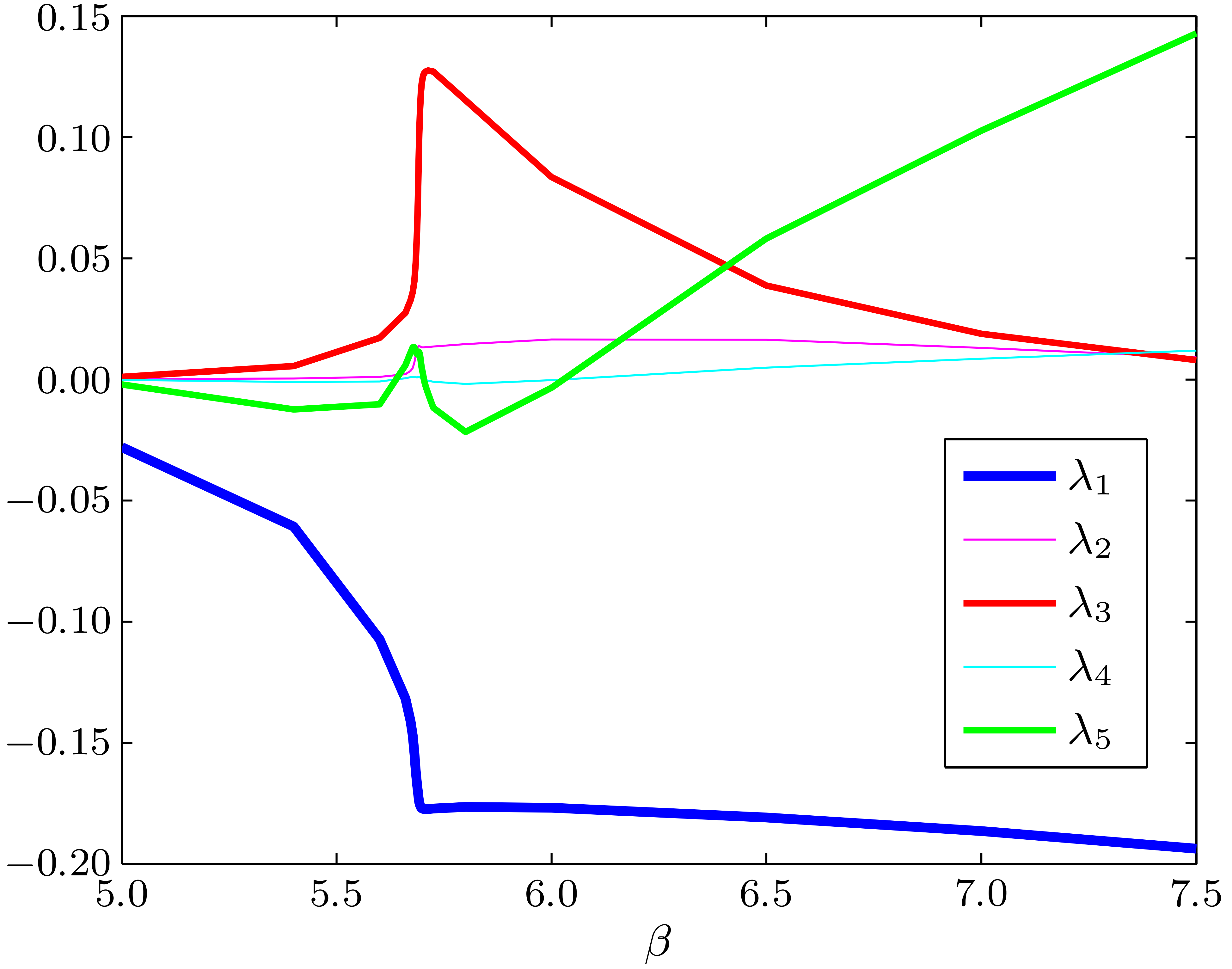
- How do we solve these equations?

IMC

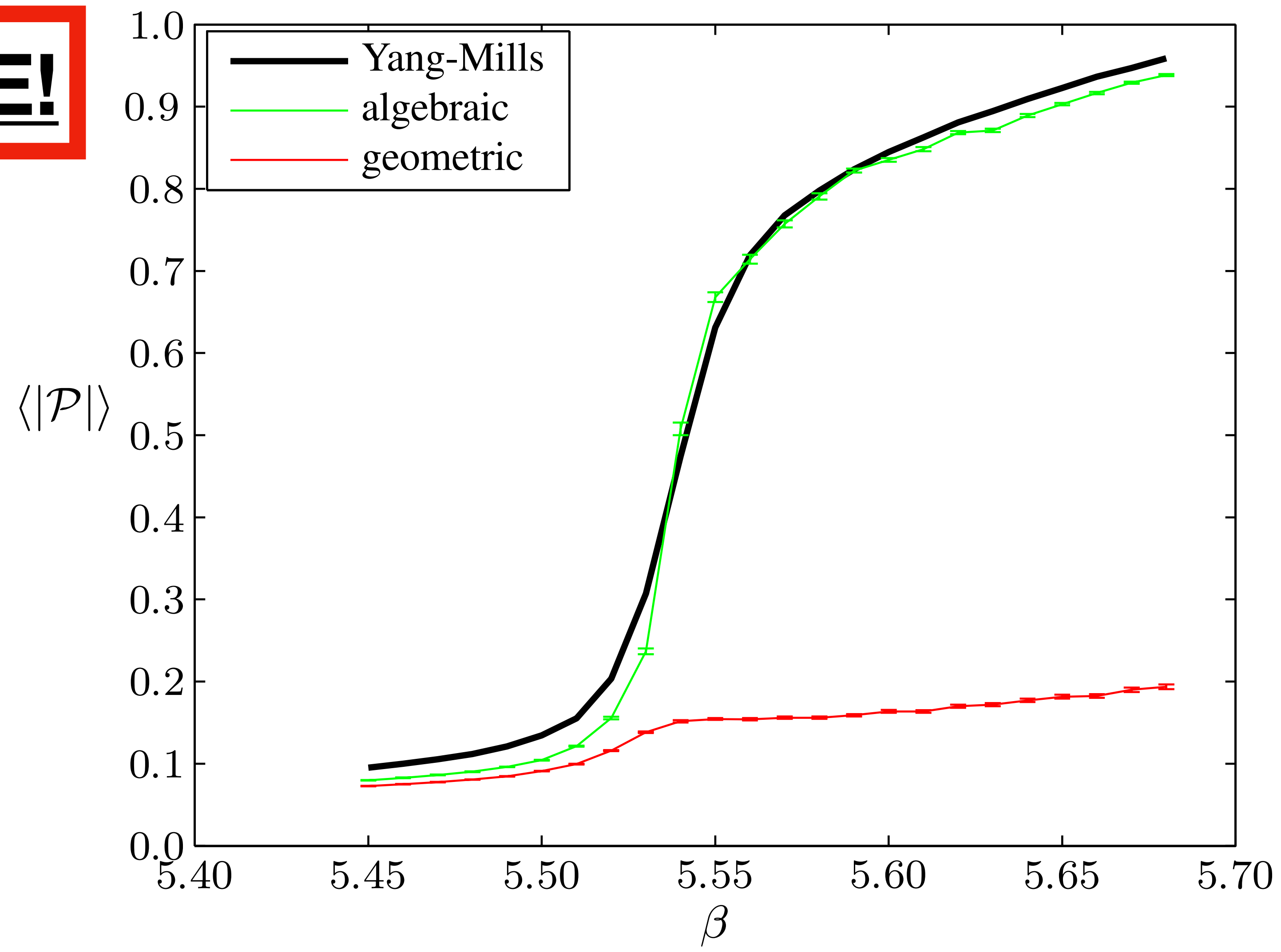
- Convert into a matrix equation: $M_{x,z}\overrightarrow{\lambda} = \overrightarrow{b}$
- Have the freedom to choose sites s.t. $d \equiv |x - z| \in \{0,1,\ldots,N_s/2\}$
- Couplings λ_i real while matrix M and vector b_i can be complex
- Generate N_{conf} configurations $\{U_\mu^{(i)}(x); i = 0,1,\ldots N_{conf}\}$ using heat bath for YM
- Convert links to Polyakov loops $\{P_x^{(i)}, P_x^{(i)*}\}$ to get an ensemble for the effective action
- Compute correlation functions and use least-squares to solve matrix equation $\forall d$
- Once we determine couplings, can compute observables with truncated action

Results (NN)

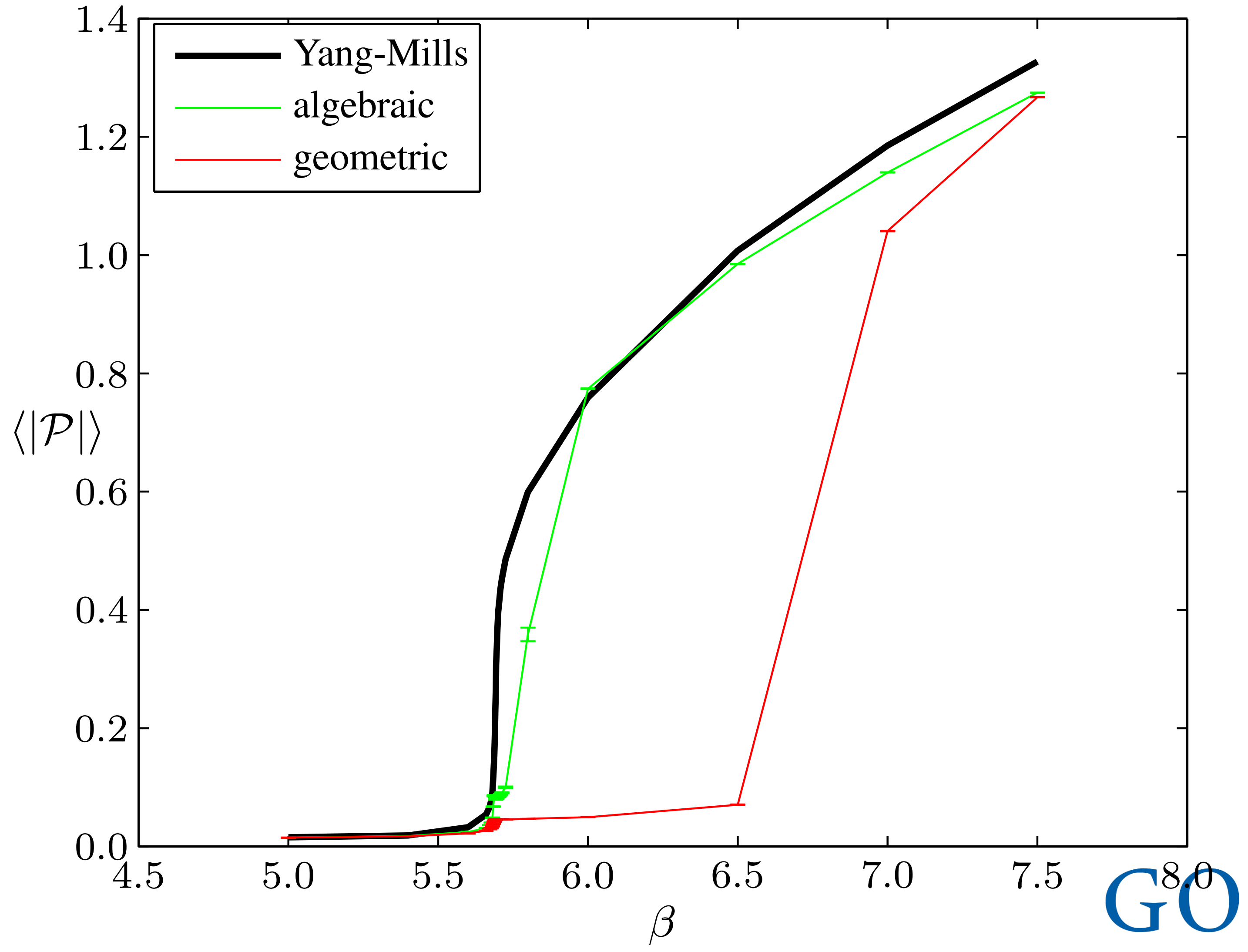
Alg vs Geometric SDE!



NN couplings vs β

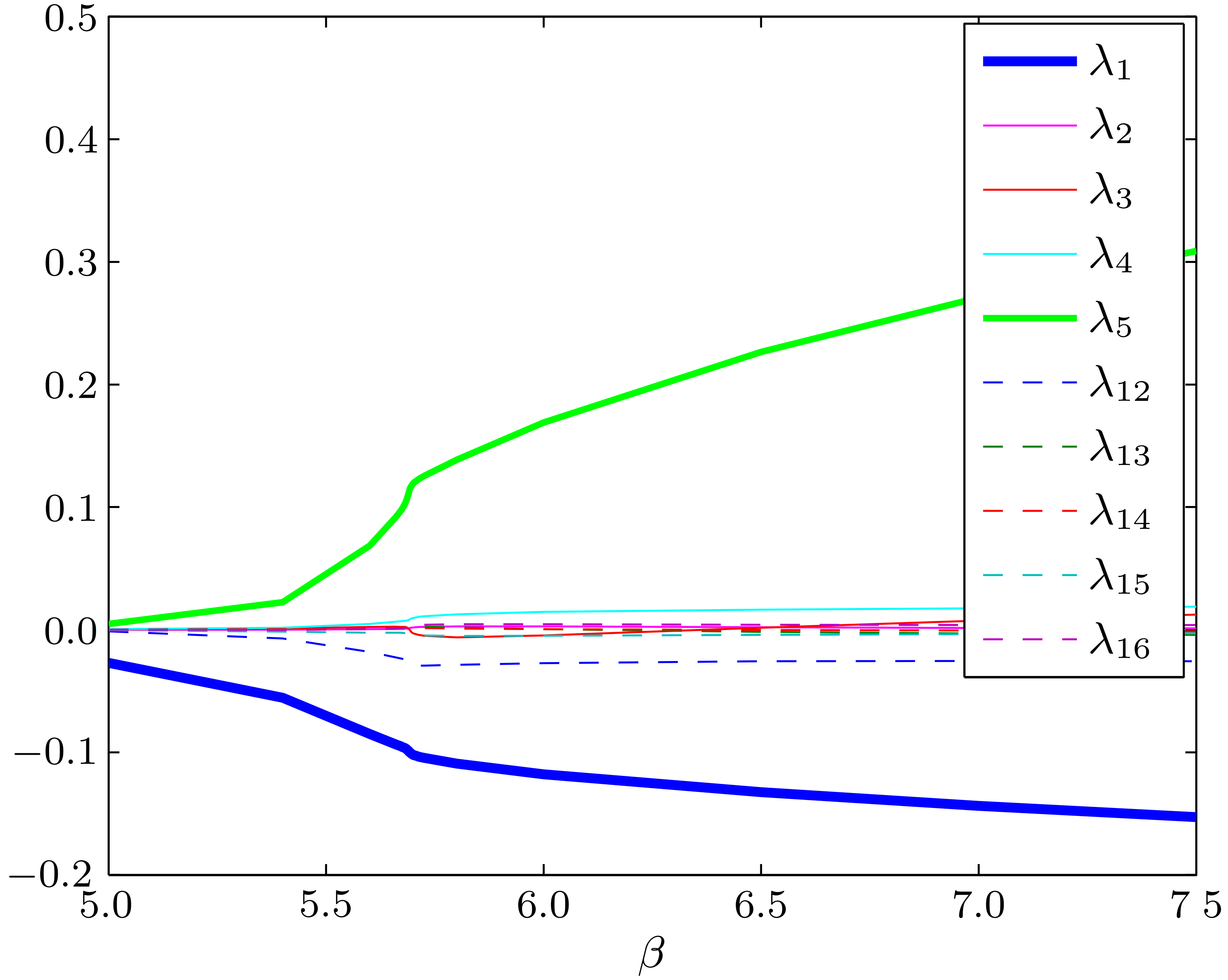


$8^3 \times 3$

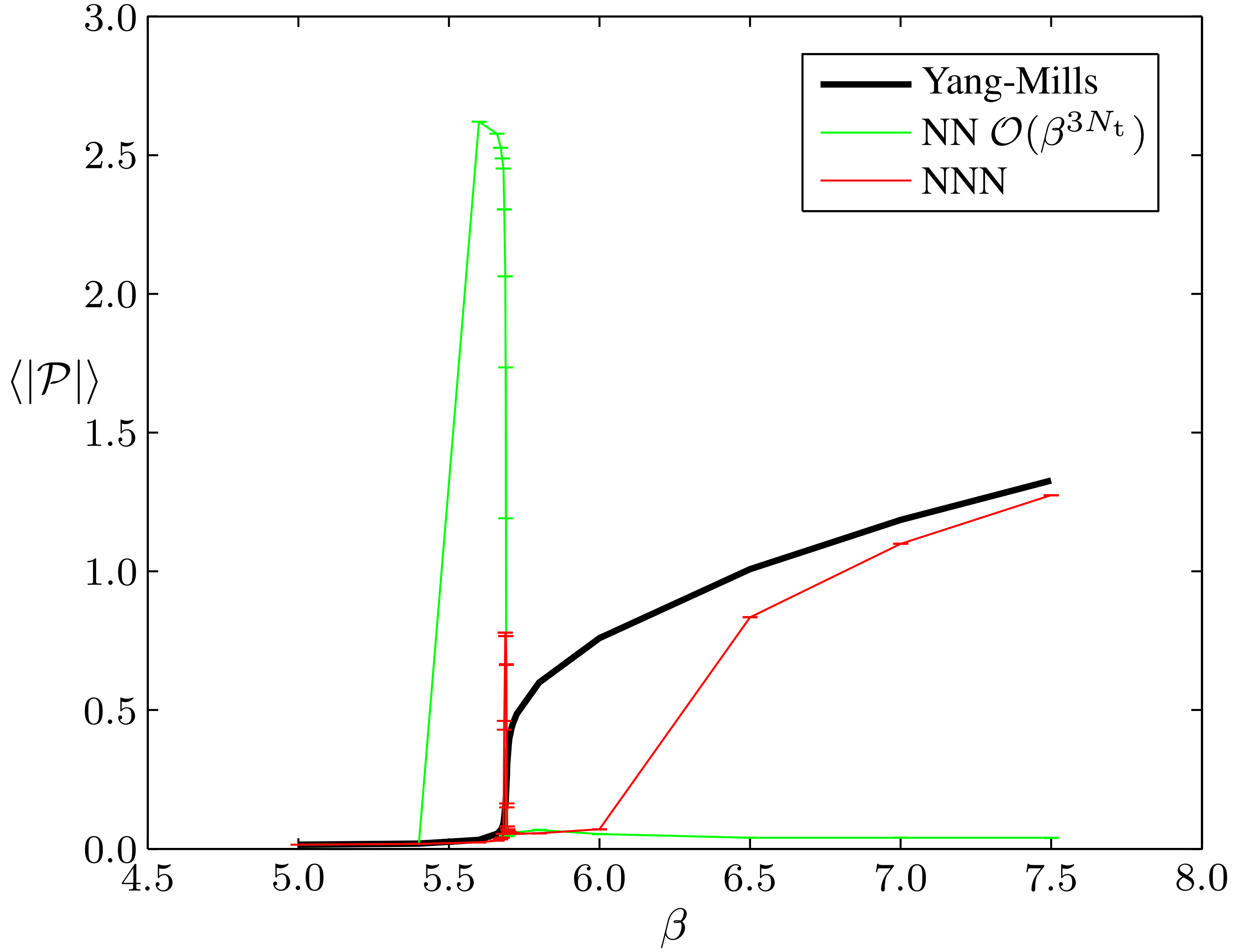


$16^3 \times 4$

Results (NN+NNN)



NN+NNN couplings vs β



fine-tuning problem!

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Conclusion

- IMC performed for SU(2) and SU(3) pure gauge theory
- Including fermions?
- Fine-tuning
- Characterizing systematic error in λ_i

NN-terms in λ basis (Backup)

$$S_3 = \sum_{\langle xy \rangle} \chi_{11}(\mathcal{P}_x)\chi_{11}(\mathcal{P}_y), \tag{A3}$$

$$S_4 = \sum_{\langle xy \rangle} (\chi_{10}(\mathcal{P}_x)\chi_{20}(\mathcal{P}_y) + \chi_{20}(\mathcal{P}_x)\chi_{10}(\mathcal{P}_y) + \text{c.c.}), \tag{A4}$$

$$S_5 = \sum_{x} \chi_{11}(\mathcal{P}_x), \tag{A5}$$

$$S_6 = \sum_{\langle xy \rangle} (\chi_{30}(\mathcal{P}_x)\chi_{03}(\mathcal{P}_y) + \text{c.c.}), \tag{A6}$$

$$S_7 = \sum_{\langle xy \rangle} (\chi_{21}(\mathcal{P}_x)\chi_{12}(\mathcal{P}_y) + \text{c.c.}), \tag{A7}$$

$$S_8 = \sum_{\langle xy \rangle} (\chi_{30}(\mathcal{P}_x)\chi_{11}(\mathcal{P}_y) + \chi_{11}(\mathcal{P}_x)\chi_{30}(\mathcal{P}_y) + \text{c.c.}), \tag{A8}$$

$$S_9 = \sum_{\langle xy \rangle} (\chi_{21}(\mathcal{P}_x)\chi_{20}(\mathcal{P}_y) + \chi_{20}(\mathcal{P}_x)\chi_{21}(\mathcal{P}_y) + \text{c.c.}), \tag{A9}$$

$$S_{10} = \sum_{\langle xv \rangle} (\chi_{21}(\mathcal{P}_x)\chi_{01}(\mathcal{P}_y) + \chi_{01}(\mathcal{P}_x)\chi_{21}(\mathcal{P}_y) + \text{c.c.}),$$

$$S_1 = \sum_{\langle xy \rangle} (\chi_{10}(\mathcal{P}_x)\chi_{01}(\mathcal{P}_y) + \text{c.c.}), \tag{A1}$$

$$S_2 = \sum_{\langle xy \rangle} (\chi_{20}(\mathcal{P}_x)\chi_{02}(\mathcal{P}_y) + \text{c.c.}), \tag{A2}$$

NNN-terms in λ basis (Backup)

$$S_{12} = \sum_{[xz]} (\chi_{10}(\mathcal{P}_x)\chi_{01}(\mathcal{P}_z) + \text{c.c.}), \tag{A12}$$

$$S_{13} = \sum_{\langle xyz \rangle} (\chi_{10}(\mathcal{P}_x)\chi_{01}(\mathcal{P}_z) + \text{c.c.})\chi_{11}(\mathcal{P}_y), \tag{A13}$$

$$S_{14} = \sum_{\langle xyz \rangle} (\chi_{10}(\mathcal{P}_x)\chi_{02}(\mathcal{P}_y)\chi_{10}(\mathcal{P}_z) + \text{c.c.}), \tag{A14}$$

$$S_{15} = \sum_{\langle xyz \rangle} (\chi_{10}(\mathcal{P}_x)\chi_{10}(\mathcal{P}_y)\chi_{10}(\mathcal{P}_z) + \text{c.c.}), \tag{A15}$$

$$S_{16} = \sum_{(xy,vw)} (\chi_{10}(\mathcal{P}_x)\chi_{01}(\mathcal{P}_y) + \text{c.c.}) \cdot (\chi_{10}(\mathcal{P}_v)\chi_{01}(\mathcal{P}_w) + \text{c.c.}). \tag{A16}$$

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