Low-Scaling G_0W_0 in the LAPW Basis

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NOMAD
NOVEL MATERIALS DISCOVERY

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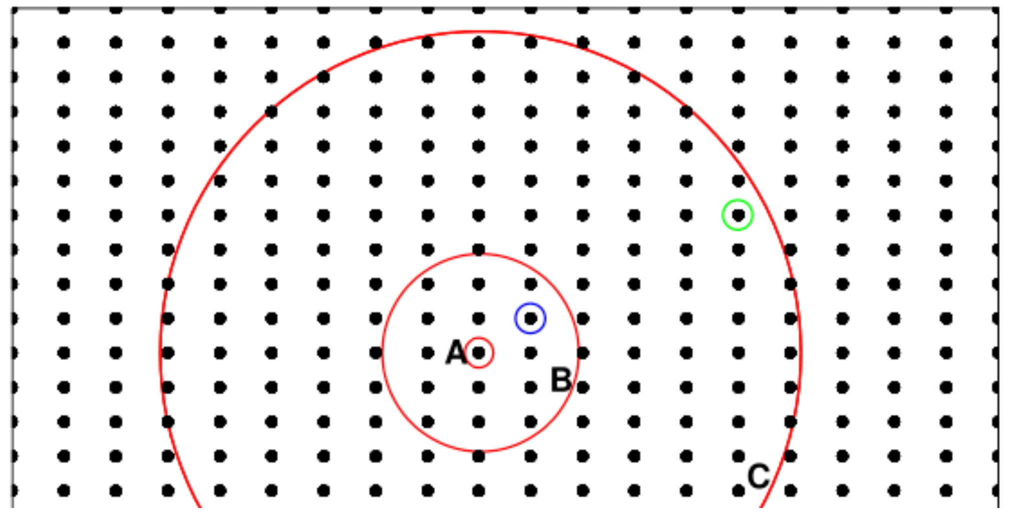
Real <-> Momentum Space - Imaginary Time [1]



- Want to choose representations/bases where quantities are constructed with matrix-matrix products, not integrals/convolutions.

- FFTs are an extremely efficient way of transforming between time-frequency and real-momentum spaces. Scale as ~ *N log(N)*

- G, W, Σ contain a lot of structure along real time/frequency axes. Can be more efficient to work in imaginary time or frequency, where the functions are smoother.

- $\Sigma \rightarrow 0$ as $|\mathbf{r}-\mathbf{r}'| \rightarrow \infty$, implying one can employ a real-space cut-off and reducing the scaling by an additional order of magnitude [2].

[1]. Rojas, H. N., Rex William Godby, and R. J. Needs. Physical review letters 74.10 (1995): 1827.

[2]. A.L. Kutepov / Computer Physics Communications 257 (2020) 107502

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Notation

Indices	Description
α, β	Atomic Sites
n	Kohn-Sham State
L	LAPW State
K	Product Basis State
τ	Img Time

Terms	Description
$Z_{\alpha L n}$	KS Coefficients (in MT region)
φ_L^α	Local Orbitals
M_K^α	Product Basis Functions
$A_{\mathbf{G}}^{\mathbf{k}n}$	KS Coefficients (in Int region)

(Real) Space - (Img) Time Method for Cubic GW

Greens function:
Band rep/imaginary time

$$G^{\mathbf{k}}_{n,n}(\tau) = \begin{cases} e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau < 0 \\ -e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau > 0 \end{cases}$$

$$G^{\mathbf{R}}_{\alpha L,\beta L'}(\tau) = \boxed{\frac{1}{N_{\mathbf{k}}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} \boxed{\sum_n Z^{\mathbf{k}}_{\alpha L n} G^{\mathbf{k}}_{n,n}(\tau) Z^{\mathbf{k}*}_{\beta L' n}}}$$

Matrix product

FFT

Greens function:
Real-space/imaginary time

Contraction over LAPW basis indices

$$\xrightarrow{\quad\quad} \sum_{LL'L''L'''}$$

$$P^{\mathbf{R}}_{\alpha K;\beta K'}(\tau)$$

Polarisability in product basis

FFT P to reciprocal space

$$\longrightarrow \quad \epsilon^{\mathbf{q}}_{\alpha K;\beta K'}(\tau)$$

Adler-Wiser Expression

Muffin Tin -Muffin Tin

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Polarisability: Muffin Tin - Muffin Tin

1. Band representation in imaginary-time

$$G^{\mathbf{k}}_{n,n}(\tau) = \begin{cases} e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau < 0 \\ -e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau > 0 \end{cases}$$

2. Band representation to real-space representation

$$G^{\mathbf{R}}_{\alpha L,\beta L'}(\tau) = \frac{1}{N_{\mathbf{k}}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}} \sum_{n} Z^{\mathbf{k}}_{\alpha L n} G^{\mathbf{k}}_{n,n}(\tau) Z^{\mathbf{k}*}_{\beta L' n}$$

3. Polarisability in product basis representation

$$P^{\mathbf{R}}_{\alpha K;\beta K'}(\tau) = -\sum_{LL''} \left\langle M^{\alpha}_{K} \mid \varphi^{\alpha}_{L}\varphi^{\alpha}_{L''}\right\rangle \times \sum_{L'} G^{\mathbf{R}}_{\alpha L';\beta L'}(\tau) \sum_{L'''} G^{\mathbf{R}}_{\alpha \mathbf{L}'';\beta L'''}(-\tau) \times \left\langle \varphi^{\beta}_{L'}\varphi^{\beta}_{L'''} \mid M^{\beta}_{K'}\right\rangle .$$

Scaling

$$(N_{At} N_{orb} N_{\mathbf{k}} N_{\tau})$$

$$[(N_{At}N_{orb})^3 N_{\mathbf{k}} + (N_{At}N_{orb})^2 N_{\mathbf{k}} \ln N_{\mathbf{k}}] N_{\tau}$$

$$[2N^3_{orb} N^{MT}_{PB} + (N_{orb} N^{MT}_{PB})^2)] N_{At} N_{\mathbf{k}} N_{\tau}$$

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(Real) Space - (Img) Time Method for Cubic GW

Greens function:
Band rep/imaginary time

$$G^{\mathbf{k}}_{n,n}(\tau) = \begin{cases} e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau < 0 \\ -e^{-\epsilon_n \tau}\delta_{nn'} & \text{if } \tau > 0 \end{cases}$$

Greens function:
reciprocal/imaginary time

$$G^{\mathbf{k}}_{\mathbf{G},\mathbf{G}'}(\tau) = \frac{1}{\Omega}\boxed{\sum_{nn'} A^{\mathbf{k}n}_{\mathbf{G}} G^{\mathbf{k}}_{nn'}(\tau) A^{*\mathbf{k}n'}_{\mathbf{G}'}}$$

Matrix product

$$G^{\mathbf{R}}_{\mathbf{rr}'}(\tau) = \boxed{\sum_{\mathbf{k}} e^{i\mathbf{kR}} \sum_{\mathbf{GG}'} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} G^{\mathbf{k}}_{\mathbf{G},\mathbf{G}'}(\tau) e^{-i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}'}}$$

Matrix products or FFTs

$$P^{\mathbf{R}}_{\mathbf{rr}'} = -\,G^{\mathbf{R}}_{\mathbf{rr}'}(\tau) G^{\mathbf{R}}_{\mathbf{rr}'}(-\tau)$$

Hadamard Product

Triple FFT to reciprocal space

$$\tilde{P}^{\mathbf{q}}_{\mathbf{GG}'}(\tau) \xrightarrow{\sum_{LL'L''L'''}} P^{\mathbf{q}}_{K,K'}(\tau)$$

Contraction over LAPW basis indices

Interstitial - Interstitial

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Polarisability: Interstitial - Interstitial

2. Band representation to reciprocal-space representation

Scaling

$$G^{\mathbf{k}}_{\mathbf{G},\mathbf{G}'}(\tau) = \frac{1}{\Omega}\sum_{nn'} A^{\mathbf{k}n}_{\mathbf{G}} G^{\mathbf{k}}_{nn'}(\tau) A^{*\mathbf{k}n'}_{\mathbf{G}'}$$

$$(N_{At}N_{orb})^3 N_{\mathbf{k}} N_\tau$$

3. Reciprocal-space representation to real-space representation

$$G^{\mathbf{R}}_{\mathbf{rr}'}(\tau) = \sum_{\mathbf{k}} e^{i\mathbf{kR}} \sum_{\mathbf{GG}'} e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{r}} G^{\mathbf{k}}_{\mathbf{G},\mathbf{G}'}(\tau) e^{-i(\mathbf{k}+\mathbf{G}')\cdot\mathbf{r}'}$$

$$(N_{At}N_{\mathbf{r}})^2 N_{\mathbf{k}} N_\tau [2\ln(N_{At}N_{\mathbf{r}}) + \ln N_{\mathbf{k}}]$$

$$P^{\mathbf{R}}_{\mathbf{rr}'} = -G^{\mathbf{R}}_{\mathbf{rr}'}(\tau) G^{\mathbf{R}}_{\mathbf{rr}'}(-\tau)$$

$$(N_{At}N_{\mathbf{r}})^2 N_{\mathbf{k}} N_\tau$$

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Polarisability: Interstitial - Interstitial

4. Real-space Polarisability to Reciprocal-space Polarisability

Scaling

$$\tilde{P}^{\mathbf{q}}_{\mathbf{G}\mathbf{G}'}(\tau) = \frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{r}} e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}\frac{1}{N_{\mathbf{r}}}\sum_{\mathbf{r}'} e^{-i(\mathbf{q})+\mathbf{G})'\mathbf{r}'}\sum_{\mathbf{R}} e^{-i\mathbf{q}\mathbf{R}} P^{\mathbf{R}}_{\mathbf{r},\mathbf{r}'}(\tau)$$

$$N_{At}^2 N_{\mathbf{r}} N_{\mathbf{k}} N_{\tau}[(N_{\mathbf{r}} + N_{PB}^{int})\ln(N_{At}N_{\mathbf{r}}) + N_{\mathbf{r}}\ln N_{\mathbf{k}}]$$

5. Reciprocal-space Polarisability to Polarisability in product basis

$$P^{\mathbf{q}}_{K,K'}(\tau)\sum_{\mathbf{G}\mathbf{G}'} = \langle M^{\mathbf{q}}_K | e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}}\rangle_{\text{Int}} \tilde{P}^{\mathbf{q}}_{\mathbf{G}\mathbf{G}'}\langle e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} | M^{\mathbf{q}}_{K'}\rangle_{\text{Int}}$$

$$(N_{At}N_{PB}^{int})^3 N_{\mathbf{k}} N_{\tau}$$

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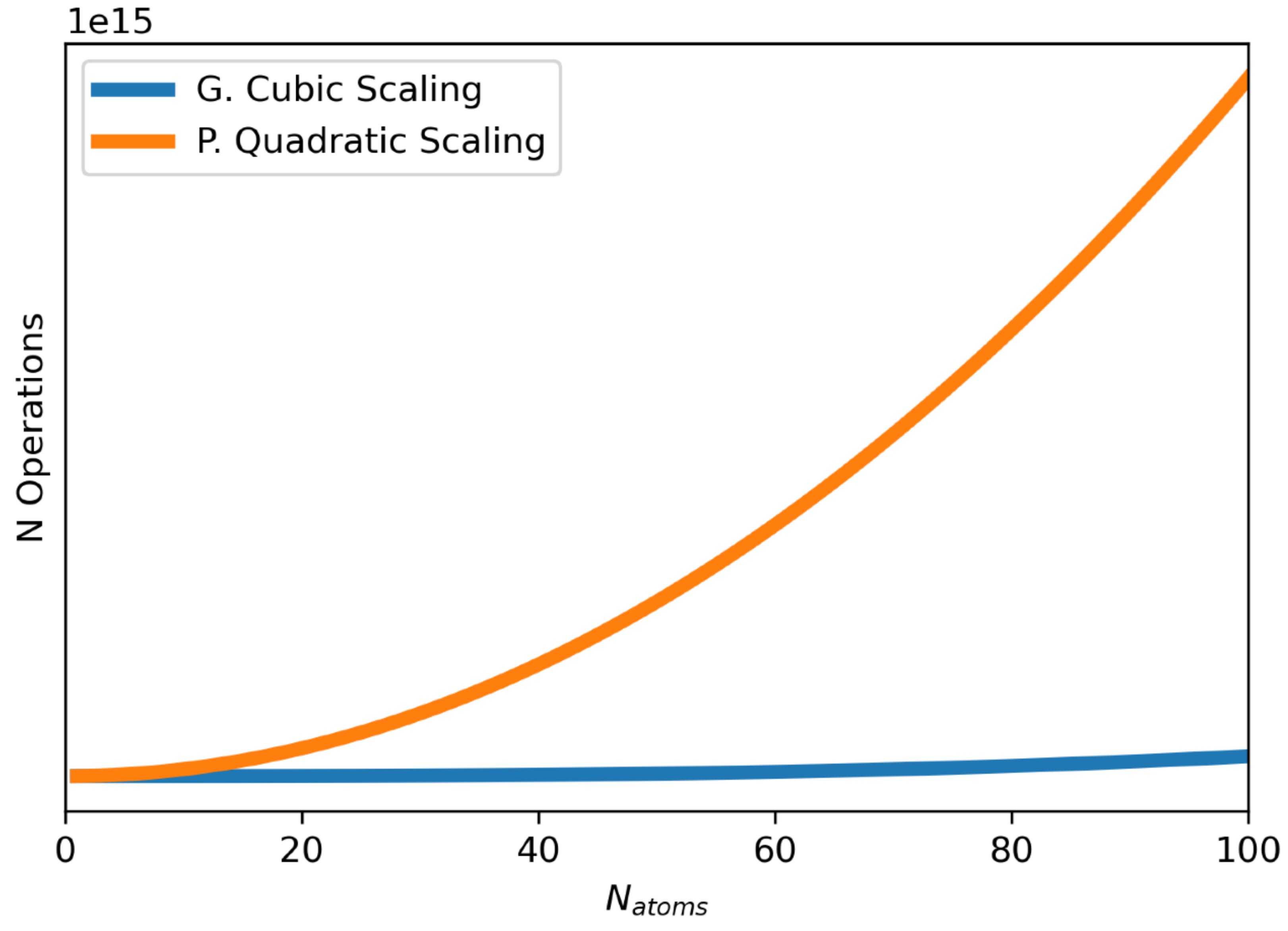
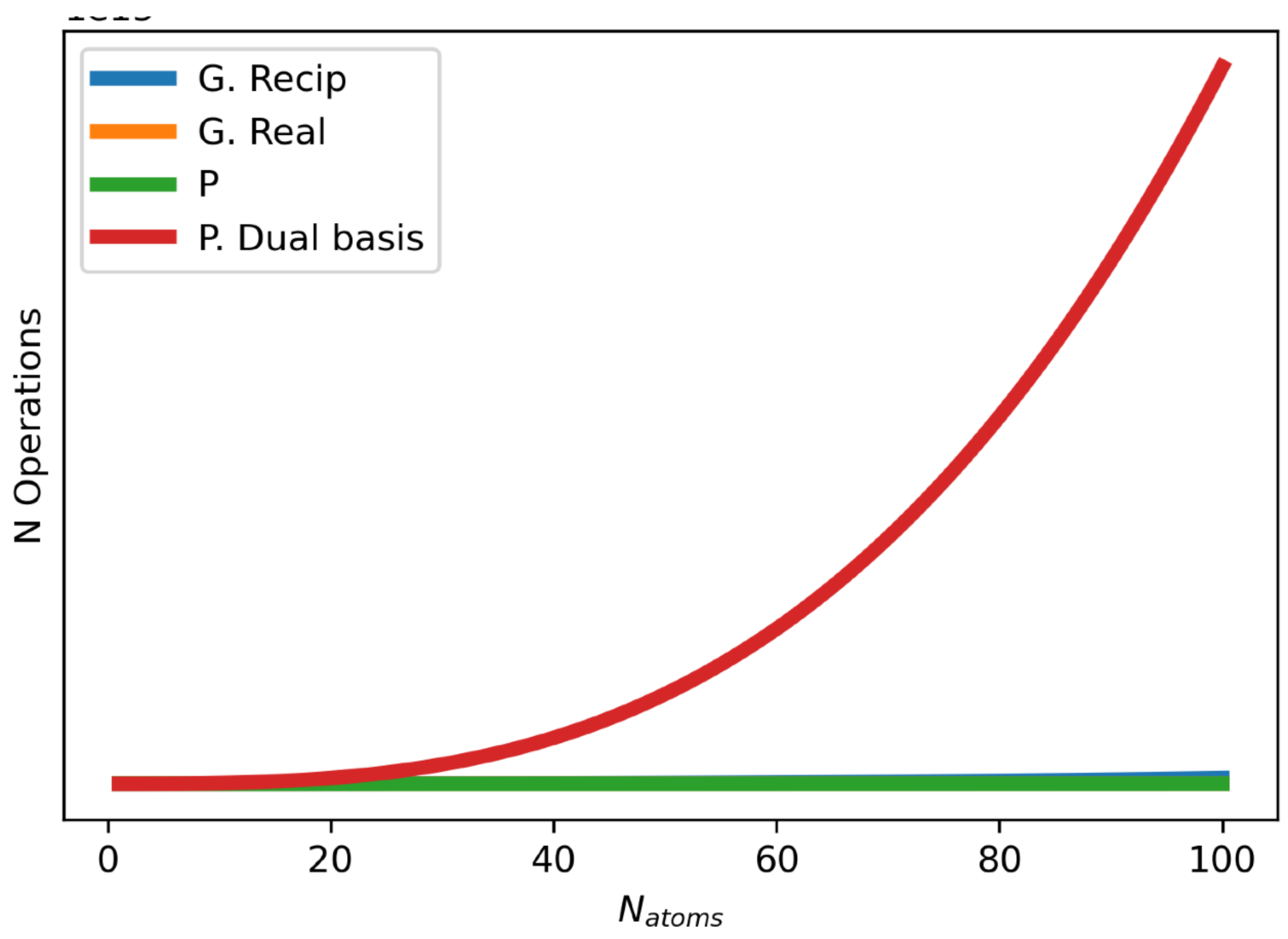
Real <-> Momentum Space, Imaginary Time in LAPW Basis
Theoretical Scaling

MT-MT



$$P^{\mathbf{R}}_{\alpha K;\beta K'}(\tau) = -\sum_{LL''} \left\langle M^{\alpha}_{K} \mid \varphi^{\alpha}_{L}\varphi^{\alpha}_{L''} \right\rangle \times \sum_{L'} G^{\mathbf{R}}_{\alpha L';\beta L'}(\tau) \sum_{L'''} G^{\mathbf{R}}_{\alpha \mathbf{L}'';\beta L'''}(-\tau) \times \left\langle \varphi^{\beta}_{L'}\varphi^{\beta}_{L'''} \mid M^{\beta}_{K'} \right\rangle .$$

Int-Int



$$P^{\mathbf{q}}_{K;K'}(\tau) = \sum_{\mathbf{GG}'} \left\langle e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} \mid M^{\mathbf{q}}_{K} \right\rangle^{*}_{\text{Int}} \widetilde{P}^{\mathbf{q}}_{\mathbf{GG}'}(\tau) \left\langle e^{i(\mathbf{q}+\mathbf{G}')\mathbf{r}'} \mid M^{\mathbf{q}}_{K'} \right\rangle_{\text{Int}} .$$

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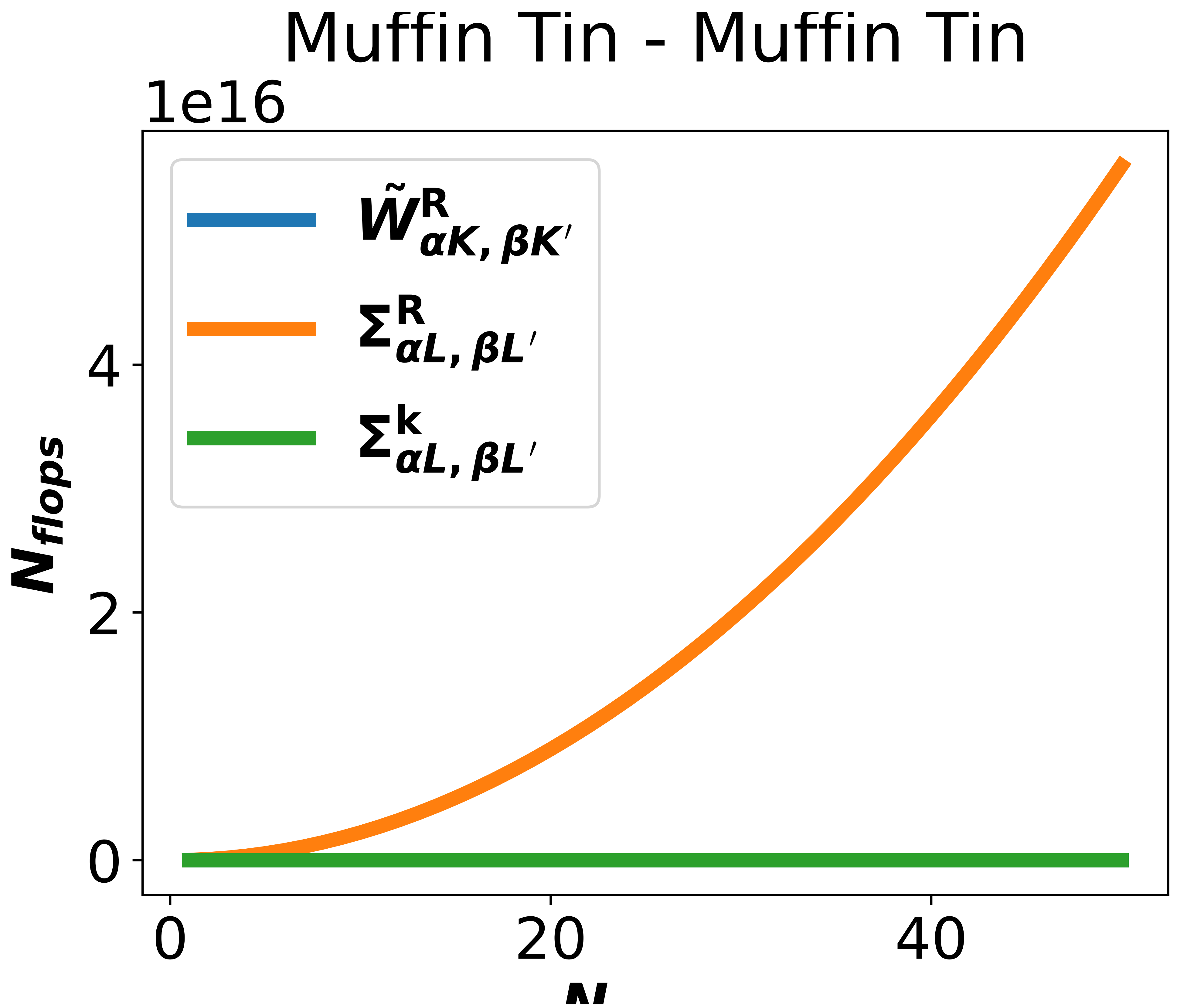
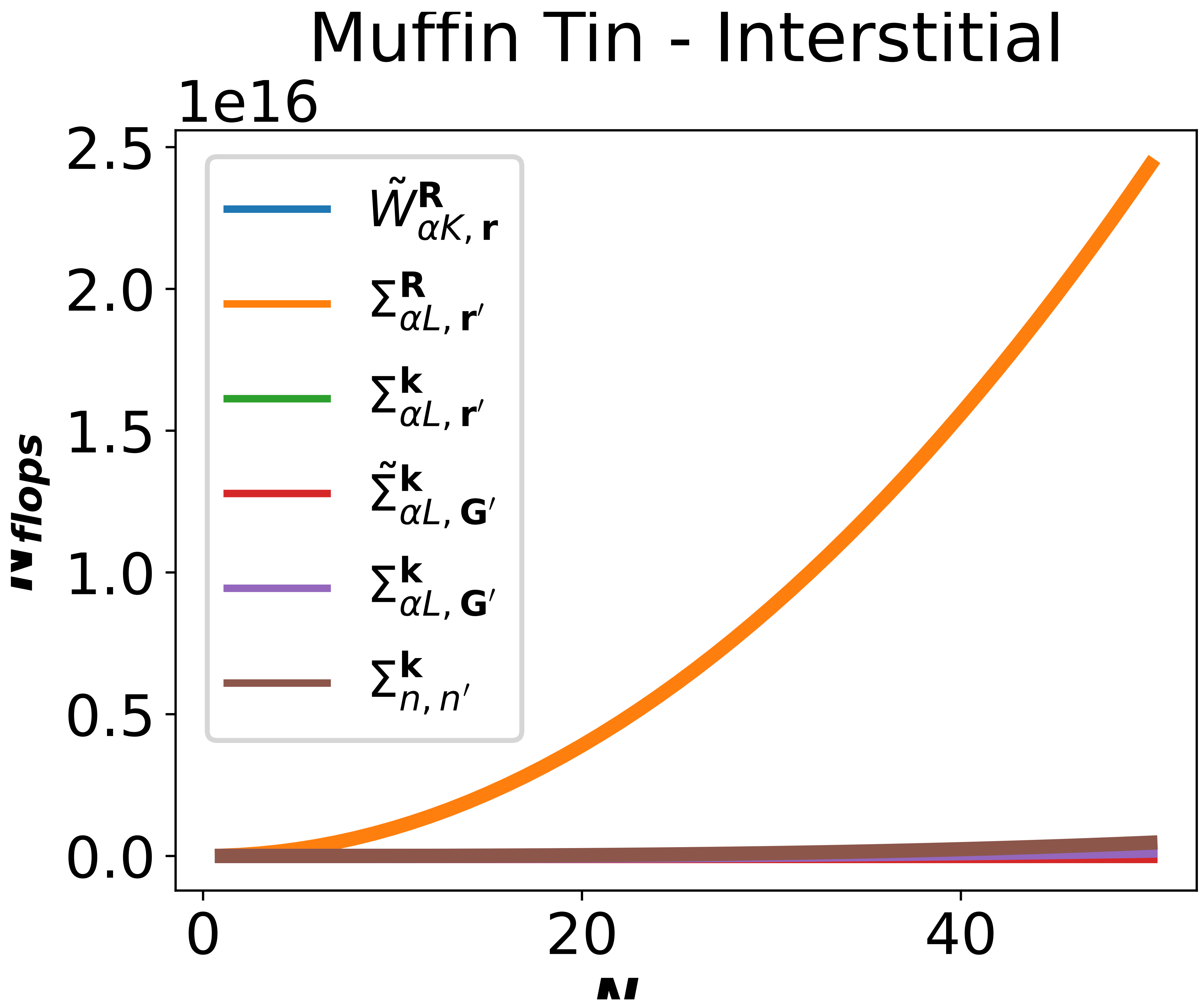
Self-Energy. Most Expensive Terms

- Same Concept, 3 terms. Flop analysis:





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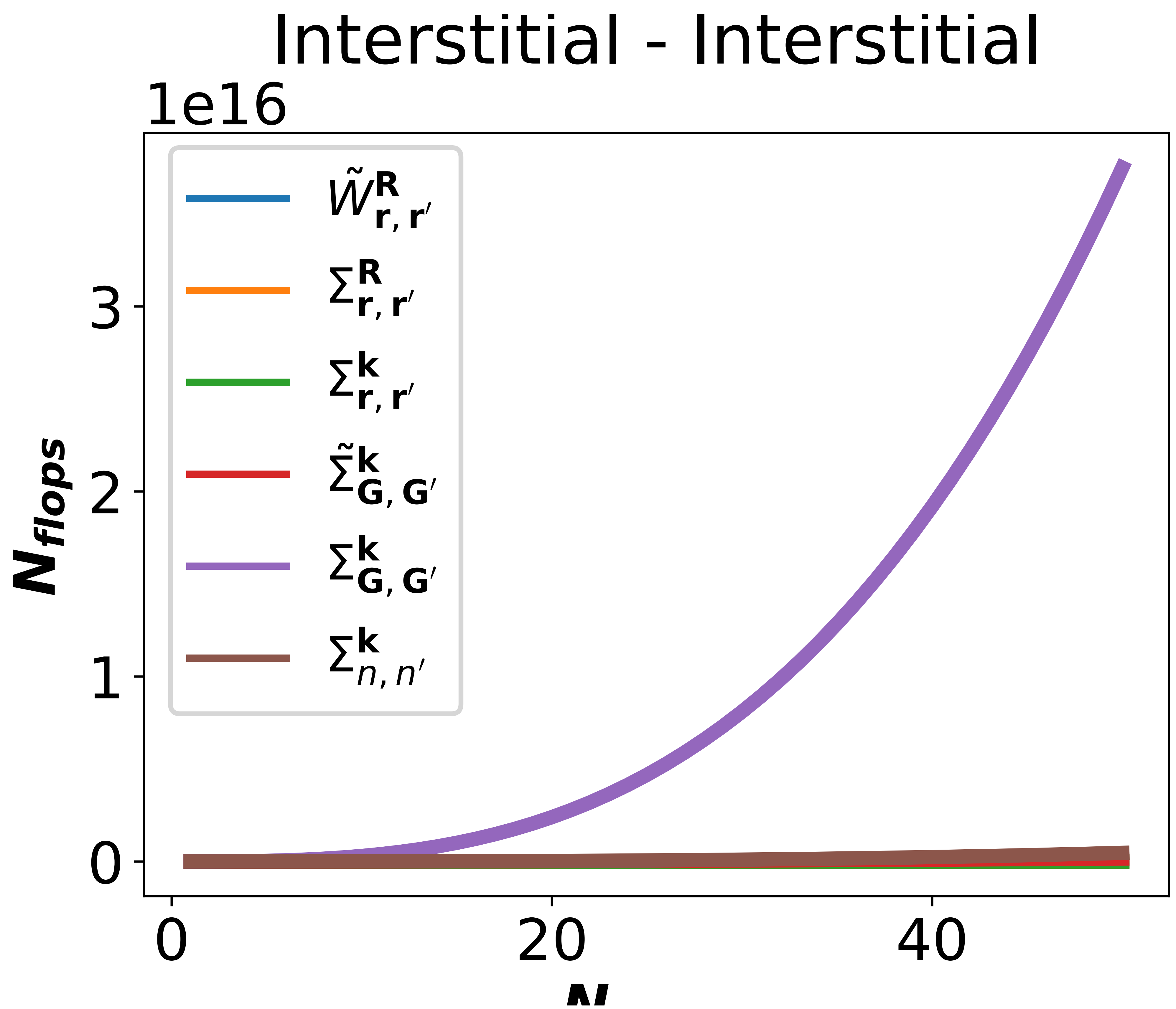

Term	Value
N_{orb}	500
N_k	1
N_r	1000
$N^{int}{}_{PB}$	200
$N^{MT}{}_{PB}$	1300
N_{tau}	30

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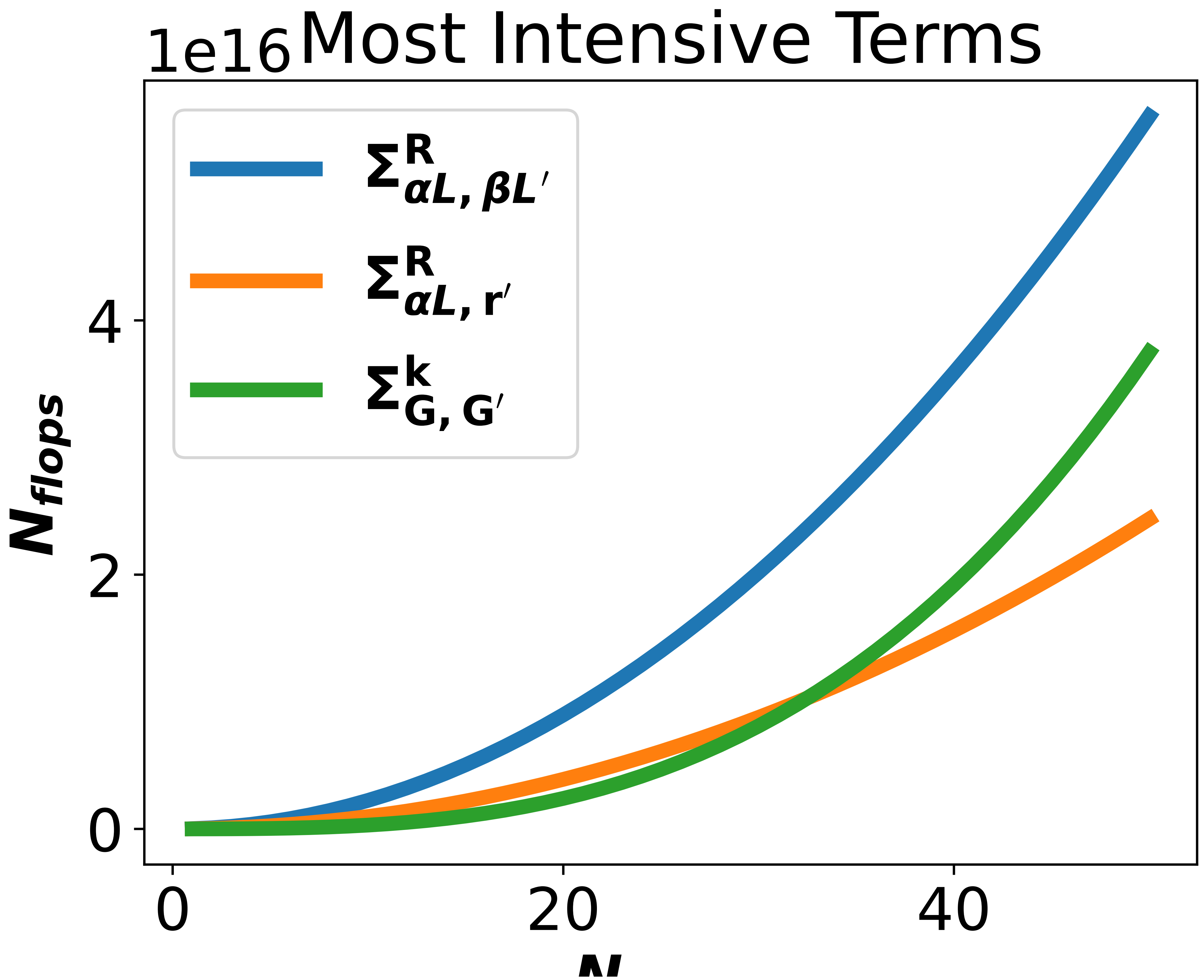
Self-Energy. Most Expensive Terms

- Same Concept, 3 terms. Flop analysis:



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Self-Energy. Most Expensive Terms

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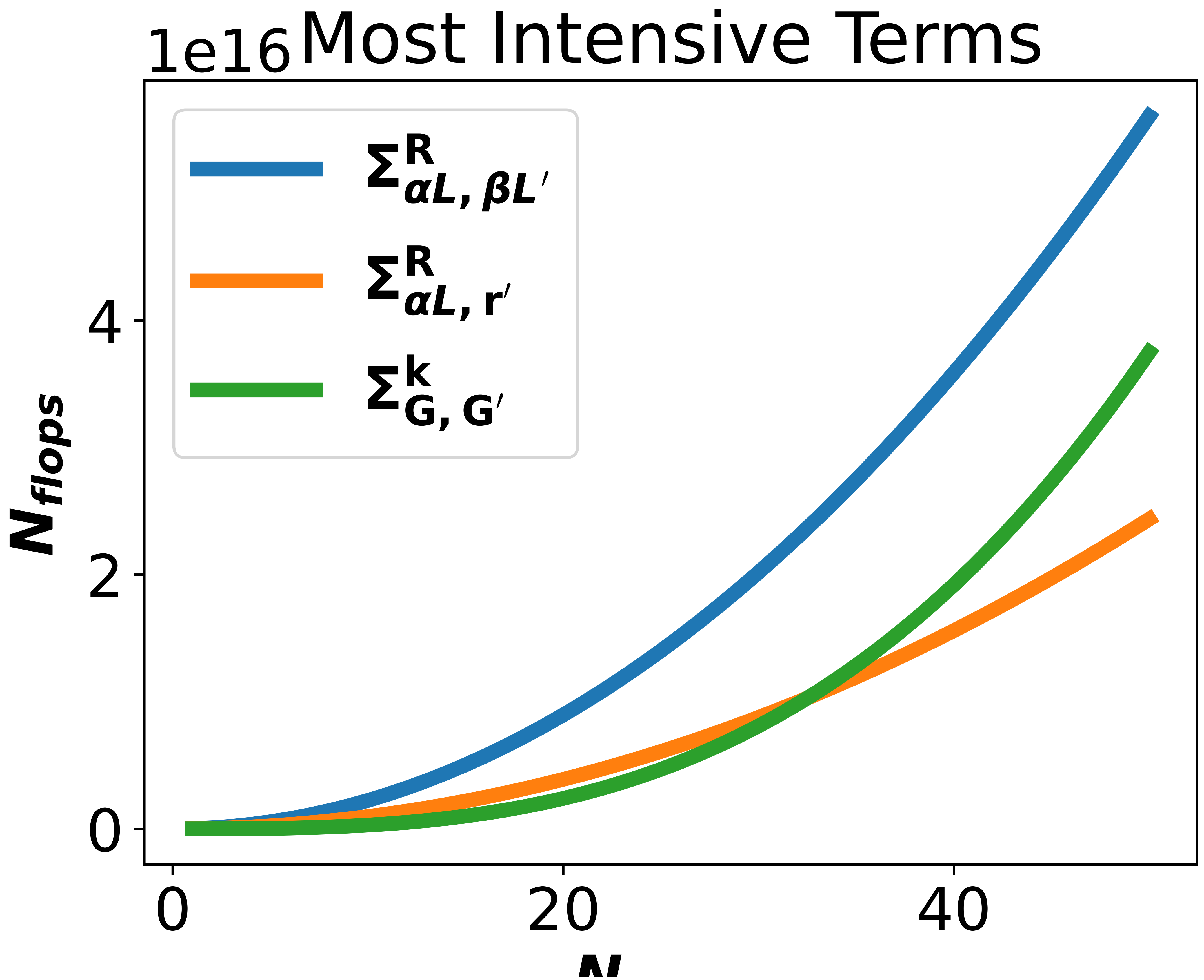

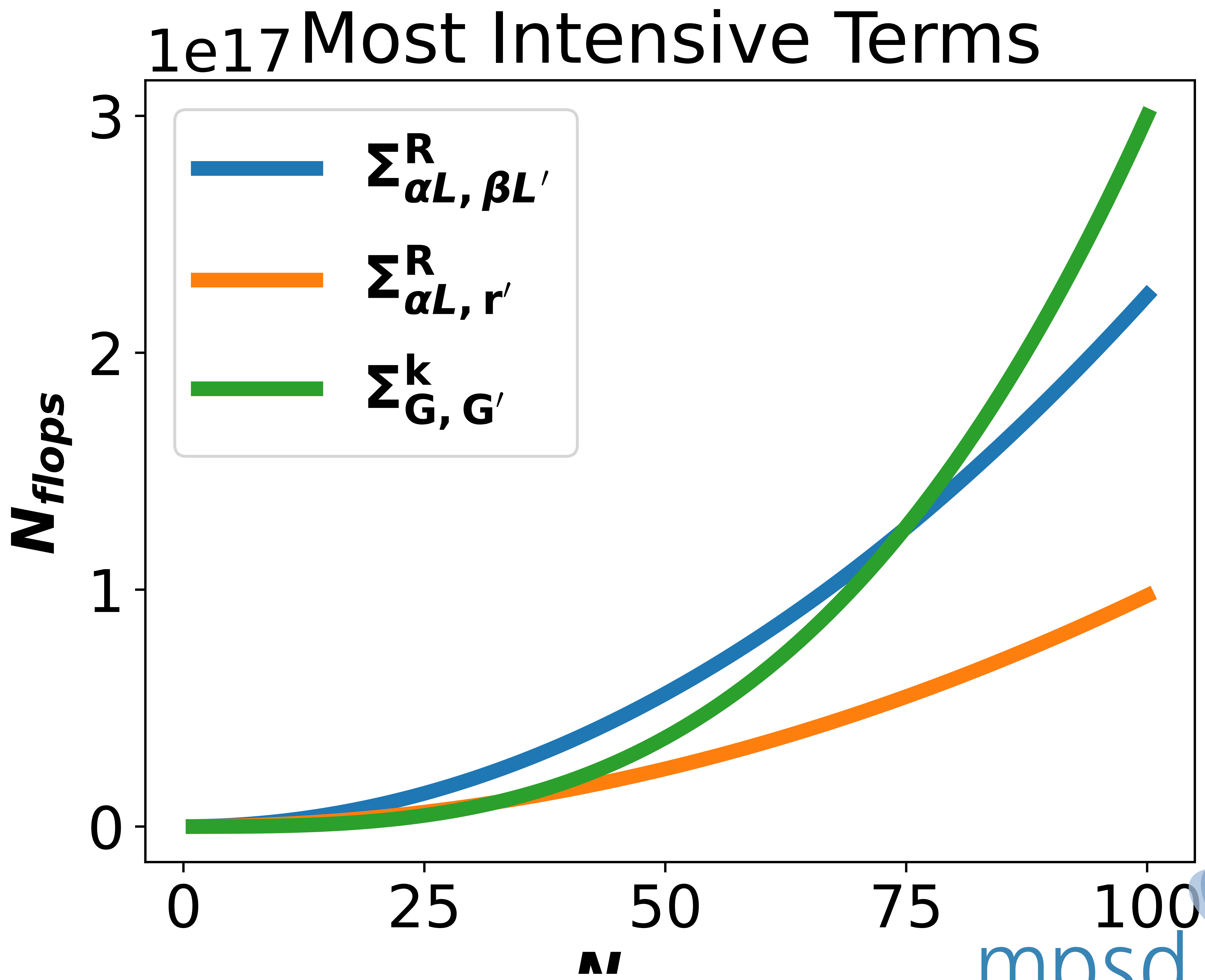

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