Accelerating Dynamical Mean-Field Calculations Using the Discrete Lehmann Representation

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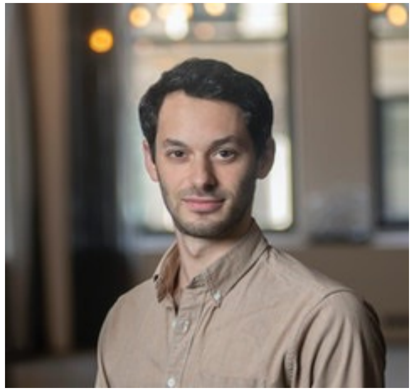

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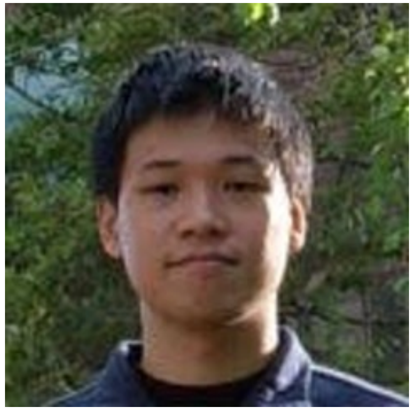
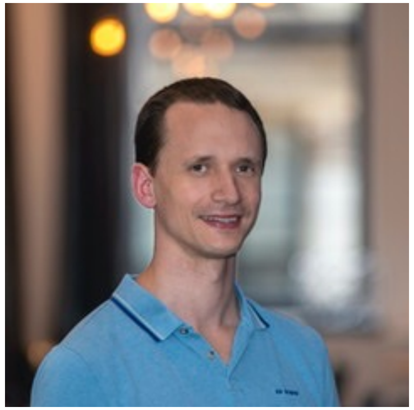


Kun Chen



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Discrete Lehmann Representation (DLR)

$$G(\tau) = -\int_{-\infty}^{+\infty} K(\tau,\omega)\rho(\omega)d\omega$$

$$K(\tau,\omega) = \frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

Physical energy cutoff
$\Lambda = \beta\omega_{max}$

→

Error ϵ

$$G(\tau) = \sum_{k=1}^{r} K(\tau,\omega_k) g_k = \sum_{k=1}^{r} e^{-\omega_k\tau}\hat{g}_k$$

Standard Discretization

DLR

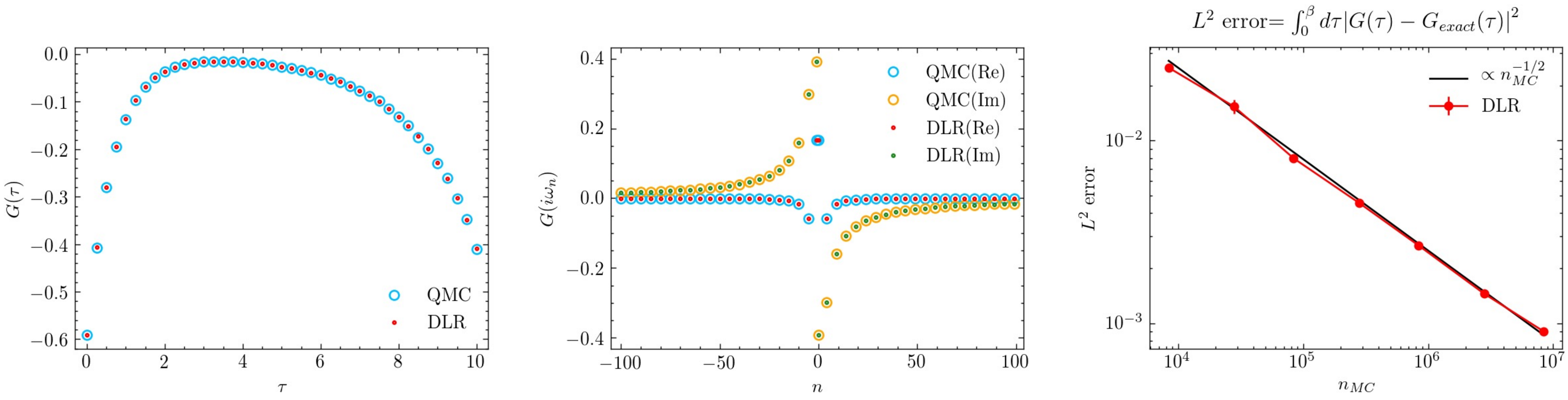
$$O(\Lambda/\epsilon) \longrightarrow O(log(\Lambda)log(1/\epsilon))$$

- DLR is a very compact representation of G obtained by low rank decomposition of Lehmann representation, another example of which is intermediate representation (IR) using SVD
- DLR selects most linearly independent $K(\tau,\omega_k)$ as basis functions
- DLR coefficients g_k can be recovered from $G(\tau_j)$ with DLR grid $\{\tau_j\}$
- Since DLR basis functions are explicit, many standard operations, e.g. Fourier transform, become explicit

Kaye, Jason, Kun Chen, and Olivier Parcollet. "Discrete Lehmann representation of imaginary time Green's functions." *arXiv preprint arXiv:2107.13094* (2021).
Shinaoka, Hiroshi, et al. "Compressing Green's function using intermediate representation between imaginary-time and real-frequency domains." *Physical Review B* 96.3 (2017): 035147.

Fitting of Noisy Green's Function

Can we fit DLR coefficients from noisy quantum Monte Carlo (QMC) data?



- In general, DLR can fit noisy data well
- DLR can capture the tail of $G(i\omega_n)$
- The error of DLR fitting follows that of QMC

triqs

Reduction of Number of Matsubara Frequencies

- Like selected $\{\tau_j\}$, DLR coefficients g_k can be recovered from $G(i\omega_{n_j})$ with selected $\{i\omega_{n_j}\}$

$$G(i\omega_n) = \sum_{k=1}^{r} K(i\omega_n, \omega_k) g_k \longrightarrow G(i\omega_{n_j})$$

$$K(i\omega_n) = (\omega + i\omega_n)^{-1}$$

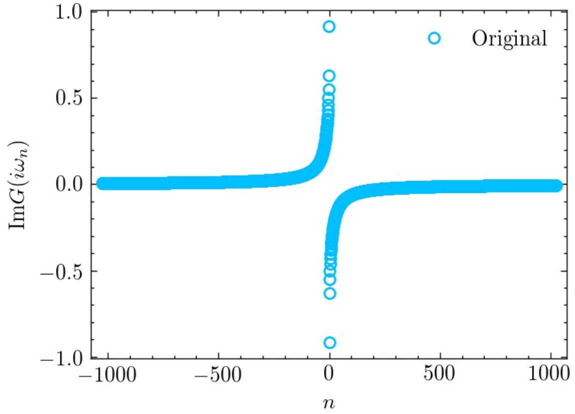
$$O(\Lambda/\epsilon) \longrightarrow O(log(\Lambda)log(1/\epsilon))$$

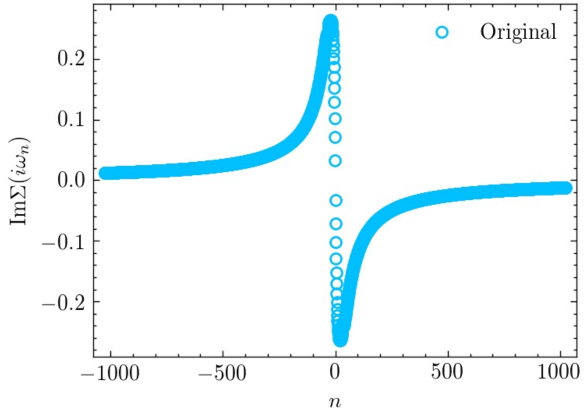
Application: Acceleration of Dyson equation solver in dynamical mean-field theory (DMFT)

- Computing k sums is a bottleneck, and the number of k sums is proportional to the number of Matsubara frequency points

$$G_{loc}(i\omega_n) = \frac{1}{N_k} \sum_{k} \left[i\omega_n - \epsilon_k + \mu - \Sigma(i\omega_n) \right]^{-1} \longrightarrow G_{loc}(i\omega_{n_j})$$

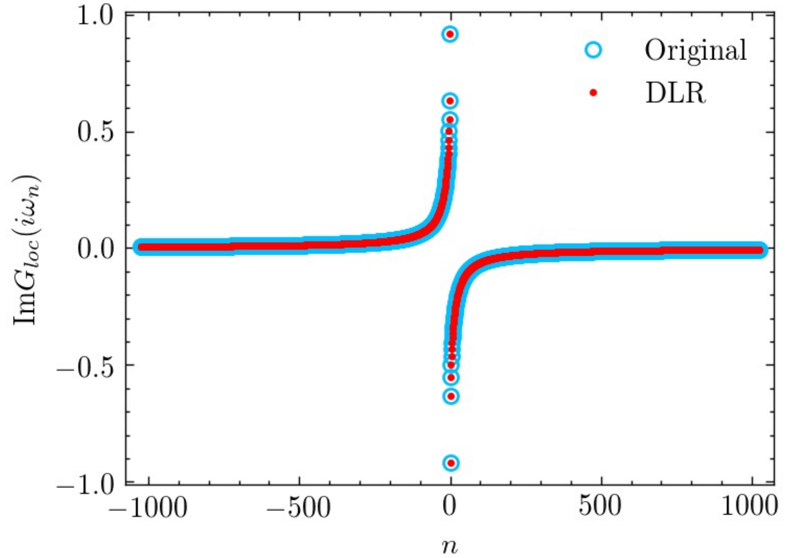
Reduction of Number of Matsubara Frequencies





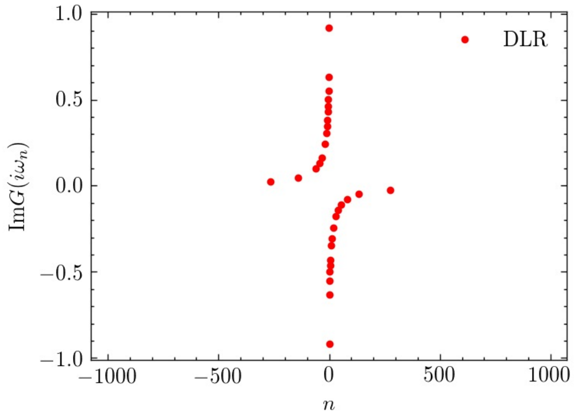
$$G_{loc}(i\omega_n) = \frac{1}{N_k}\sum_k [i\omega_n - \epsilon_k + \mu - \Sigma(i\omega_n)]^{-1}$$

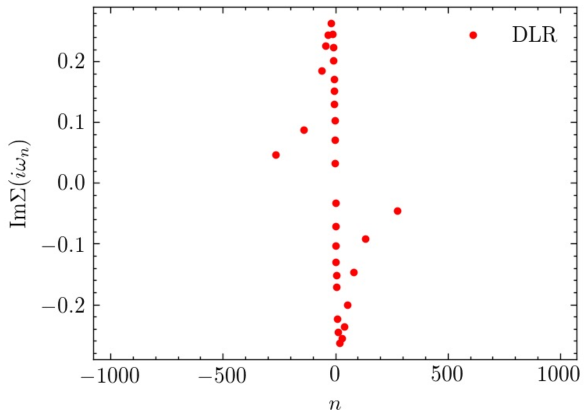
$$\Sigma(i\omega_n) = \mathcal{G}^{-1}(i\omega_n) - G^{-1}_{imp}(i\omega_n)$$



$$\mathbf{2050} \text{ frequencies} \xrightarrow{DLR} \mathbf{30} \text{ frequencies}$$

$$\Sigma(i\omega_{n_j}) = \mathcal{G}^{-1}(i\omega_{n_j}) - G^{-1}_{imp}(i\omega_{n_j})$$





$$G_{loc}(i\omega_{n_j}) = \frac{1}{N_k}\sum_k [i\omega_{n_j} - \epsilon_k + \mu - \Sigma(i\omega_{n_j})]^{-1}$$

Conclusions & Future Work

Conclusions

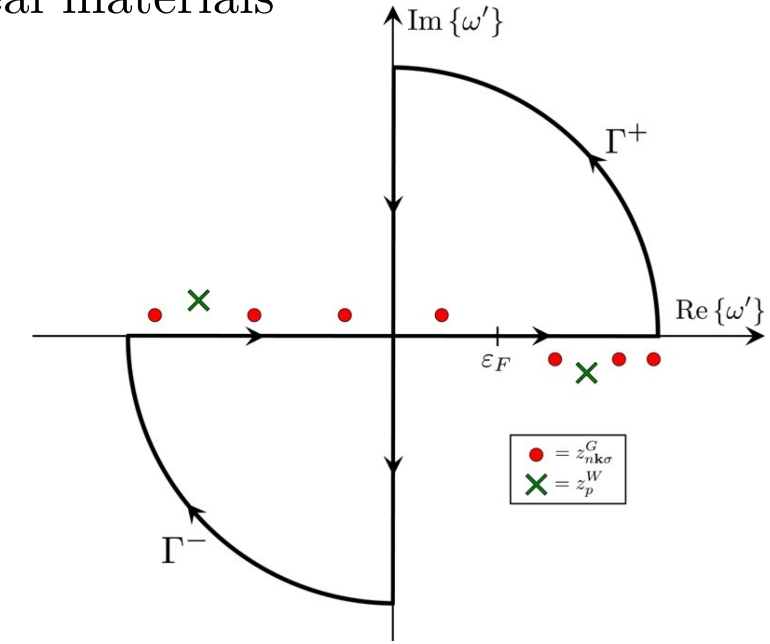
- Noisy Green's function can be well fitted by DLR
- Dyson equation solver in DMFT can be accelerated by DLR

Future Work

- A robust implementation for calculations of real materials
- Apply DLR to the GW approximation

the GW self-energy

$$\Sigma(\omega) = i\int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} G(\omega + \omega') W(\omega')$$



Govoni, Marco, and Giulia Galli. "Large scale GW calculations." *Journal of chemical theory and computation* 11.6 (2015): 2680-2696.

Discrete Lehmann Representation (DLR)

$$G(\tau) = -\int_{-\infty}^{+\infty} K(\tau,\omega)\rho(\omega)d\omega$$

$$K(\tau,\omega) = \frac{e^{-\omega\tau}}{1+e^{-\beta\omega}}$$

$\omega \to \beta\omega$

$\tau \to \tau/\beta$

Physical energy cutoff

$\Lambda = \beta\omega_{max}$

$$G(\tau) = -\int_{-\Lambda}^{+\Lambda} K(\tau,\omega)\rho(\omega)d\omega$$

$$K(\tau,\omega) = \frac{e^{-\omega\tau}}{1+e^{-\omega}}$$

Energy resolution ϵ

DLR

$$G(\tau) = \sum_{k=1}^{r} K(\tau,\omega_k)g_k$$

$$K(\tau,\omega_k) = \frac{e^{-\omega\tau}}{1+e^{-\omega}}$$

$$G(i\omega_n) = \sum_{k=1}^{r} K(i\omega_n,\omega_k)g_k$$

$$K(i\omega_n,\omega_k) = \frac{1}{\omega_k + i\omega_n}$$

1. $G(\tau)$ is represented by a simple basis set expansion, depending on Λ and ϵ only. The number of basis functions r scales as $O(log(\Lambda)log(1/\epsilon))$ instead of $O(\Lambda/\epsilon)$
2. FFT between $G(\tau)$ and $G(i\omega_n)$ can be simpily done analytically
3. Instead of sparse sampling, $\{\tau_j\}$ and $\{i\omega_{n_j}\}$ could be simply obtained, with which we can recover DLR coefficients g_k

Dynamical Mean-Field Theory (DMFT)

$$\mathcal{G}(i\omega_n) \xrightarrow{FFT} \mathcal{G}(\tau)$$

$$\mathcal{G}(\tau) \xrightarrow{CTQMC} G_{imp}(\tau)$$

$$G_{imp}(\tau) \xrightarrow{FFT} G_{imp}(i\omega_n)$$

$$\Sigma(i\omega_n) = \Sigma_{imp}(i\omega_n) = \mathcal{G}^{-1}(i\omega_n) - G^{-1}_{imp}(i\omega_n)$$

$$G_{loc}(i\omega_n) = \frac{1}{N_k}\sum_k \left[i\omega_n - \epsilon_k + \mu - \Sigma(i\omega_n)\right]^{-1}$$

$$\mathcal{G}(i\omega_n) = \left[G^{-1}_{loc}(i\omega_n) + \Sigma(i\omega_n)\right]^{-1}$$

Initial $\Sigma(i\omega_n)$

DLR for DMFT

$$\mathcal{G}(i\omega_{n_j}) \xrightarrow{DLR} \mathcal{G}(\tau)$$

$$\mathcal{G}(\tau) \xrightarrow{CTQMC} G_{imp}(\tau)$$

$$G_{imp}(\tau) \xrightarrow{DLR} G_{imp}(i\omega_{n_j})$$

$$\mathcal{G}(i\omega_{n_j}) = [G_{loc}^{-1}(i\omega_{n_j}) + \Sigma(i\omega_{n_j})]^{-1}$$

$$\Sigma(i\omega_{n_j}) = \Sigma_{imp}(i\omega_{n_j}) = \mathcal{G}^{-1}(i\omega_{n_j}) - G_{imp}^{-1}(i\omega_{n_j})$$

$$G_{loc}(i\omega_{n_j}) = \frac{1}{N_k}\sum_k [i\omega_{n_j} - \epsilon_k + \mu - \Sigma(i\omega_{n_j})]^{-1}$$

Initial $\Sigma(i\omega_{n_j})$