1 $G(\tau)$

See akiss notes 2.4.

$$G(\tau) = -\left\langle \frac{1}{\beta}\sum_{ij}^{k} \left(\Delta^{(k)}\right)^{-1}_{ji} \delta(\tau, \tau'_i - \tau_j) \right\rangle_{MC} = -\left\langle \frac{1}{\beta}\sum_{ij}^{k} M^{(k)}_{ji} \delta(\tau, \tau'_i - \tau_j) \right\rangle_{MC}$$

To reduce noise and save memory, split β in to fine grids `N_TAU` and bin data. Note that for small number of `N_TAU`, the Fourier transform back to Matsubara frequency may be inaccurate.

2 $G(i\omega)$

Fourier transform each contribution to Green's function:

$$G(i\omega) = -\langle \frac{1}{\beta}\sum_{i,j} \exp^{i\omega(\tau'_j - \tau_j)} M_{ji} \rangle_{MC}$$

When compiling, define `-DMEASURE_GIO` to enable this measurement. Noisy at high frequencies.

3 Using Legendre Polynomials

To reduce high frequency noise, one can use a set of Legendre polynomials as basis and measure the coefficients. See arxiv:1104.32115.

$$G_l = \sqrt{2l+1}\int_0^\beta d\tau P_l(x(\tau)) G(\tau)$$

In CTHYB:

$$G_l = -\frac{\sqrt{2l+1}}{\beta}\left\langle \sum_{ij} M_{ji}\tilde{P}_l(\tau'_i - \tau_j) \right\rangle_{MC}$$

Where

$$\tilde{P}(\tau) = \begin{cases} P_l(x(\tau)) & \tau > 0 \\ -P_l(x(\tau+\beta)) & \tau < 0 \end{cases}$$

and

$$x(\tau) = 2\tau/\beta - 1$$

To restore $G(\tau)$ or $G(i\omega)$ from the measured set of coefficients,

$$G(\tau) = \sum_{l\geq 0} \frac{\sqrt{2l+1}}{\beta} P_l(x(\tau)) G_l$$

and

$$G(i\omega) = \sum_{l\geq 0} G_l \frac{\sqrt{2l+1}}{\beta} \int_0^\beta \exp^{i\omega_n\tau} P_l(x(\tau)) = \sum_{l\geq 0} T_{nl} G_l$$

Where

$$T_{nl} = (-1)^n i^{l+1} \sqrt{2l+1} j_l \left(\frac{(2n+1)\pi}{2} \right)$$

and $j_l(z)$ are spherical Bessel functions. Note that in the procedure, no model-guided Fourier transform is used.

By setting an appropriate cut-off at number of Legendre series, high frequency noise is filtered. TRIQS used 80.

When compiling the code, use `-DMEASURE_LEG` to enable this measurement.