Implementation of the cumulant approximation

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In this note, I discuss the details on the implementation of the cumulant approximation. The implementation in Julia is available in `https://github.com/jaemolihm/cumulant`.

We suppose the following quantities are already given: (i) ε, the bare eigenvalue plus the static self-energy, and (ii) $\Sigma(\omega)$, the retarded self-energy minus the static part, satisfying the Kramers–Kronig relation

$$\mathrm{Re}\,\Sigma(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\mathrm{d}\omega'\,\frac{\mathrm{Im}\,\Sigma(\omega')}{\omega'-\omega}\,. \tag{1}$$

Let us first consider the retarded cumulant. The Landau form of the cumulant function reads [1]

$$C^{\mathrm{R}}(t) = \int_{-\infty}^{\infty}\mathrm{d}\omega\,\beta(\omega+\varepsilon)\frac{e^{-i\omega t}-1+i\omega t}{\omega^2}\,, \tag{2}$$

where

$$\beta(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,\Sigma(\omega)\,. \tag{3}$$

The retarded cumulant Green function reads

$$G^{\mathrm{R,\,cum}}(\omega) = -i\int_{-\infty}^{\infty}\mathrm{d}t\,\Theta(t)e^{i(\omega-\varepsilon)t}e^{C^{\mathrm{R}}(t)}. \tag{4}$$

Ideally, $C^{\mathrm{R}}(t)$ should be calculated using Eq. (2) on a dense, wide grid of time points. However, such a calculation could be time consuming. To reduce computational cost, we utilize the fact that in the limit of large t,

$$\lim_{t\to\infty} C^{\mathrm{R}}(t) = -i\Sigma(\varepsilon)t + \left.\frac{\mathrm{d}\Sigma(\omega)}{\mathrm{d}\omega}\right|_{\omega=\varepsilon} \tag{5}$$

holds. (See App. A for the proof.) We explicitly evaluate the integral Eq. (2) only for short times, and use the asymptotic form Eq. (5) to extrapolate the cumulant function to long times. The workflow for the calculation is as follows (see function `run_cumulant_retarded`).

1. Calculate $C^{\mathrm{R}}(t)$ on a (relatively) coarse, short time grid using Eq. (2). (We use the analytic form of Σ if known; otherwise we use linear interpolation.)
2. Subtract the linear asymptotic form Eq. (5)
3. Linearly interpolate the remainder to a denser, long time grid (fill zeros beyond the short time grid)
4. Add back the linear asymptotic form Eq. (5) on the dense grid.
5. Evaluate the Green's function with Eq. (4), using the dense grid cumulant function and fast Fourier transformation.

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Note that it is important to evaluate the exponential in the time domain and then Fourier transform to frequencies. We find that evaluating Eq. (4) via a repeated convolution with C^{R} may lead to numerical problems and is hard to converge. A possible cause is that $C^{\mathrm{R}}(t)$ in the long-time limit is linearly divergent. Instead, the exponential form $e^{C^{\mathrm{R}}(t)}$ exponentially decays to zero if $\operatorname{Im}\Sigma(\varepsilon) \neq 0$, and in the worst case becomes a finite oscillatory function. Thus, its Fourier transformation yields well-behaved results.

The time-ordered cumulant satisfies

$$C^{\pm}(t) = \int_{-\infty}^{\infty} d\omega \beta^{\pm}(\omega+\varepsilon) \frac{e^{-i\omega t} - 1 + i\omega t}{\omega^2}\,, \tag{6}$$

where

$$\beta^{\pm}(\omega) = \beta(\omega)\Theta[\pm(\mu-\omega)]\,. \tag{7}$$

Thus, the time-ordered cumulant function can be computed similarly by replacing β with $\beta^{\pm}$, and recomputing the corresponding real part using the Kramers–Kronig relation.

Appendix A: Proof of the asymptotic limit [Eq. (5)]

Using

$$\begin{aligned}
\lim_{t\to\infty} \frac{e^{-i\omega t} - 1}{\omega} = -i \lim_{t\to\infty} \int_0^t e^{-i\omega t'} \mathrm{d}t' &= -i \lim_{t\to\infty} \lim_{\eta\to 0^+} \int_0^t e^{-i\omega t'} e^{-\eta t'} \mathrm{d}t' \\
&= -i \lim_{\eta\to 0^+} \int_0^\infty e^{-i(\omega - i\eta)t'} \mathrm{d}t' \\
&= -\lim_{\eta\to 0^+} \frac{1}{\omega - i\eta} \\
&= -\mathcal{P}\frac{1}{\omega} - i\pi\delta(\omega)\,,
\end{aligned} \tag{A1}$$

we find

$$\lim_{t\to\infty} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \beta(\omega+\varepsilon) \frac{e^{-i\omega t} - 1}{\omega} = -\mathcal{P}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\beta(\omega+\varepsilon)}{\omega} - i\pi\beta(\varepsilon) = \Sigma(\varepsilon)\,. \tag{A2}$$

The principal value term gives the real part of the self-energy via the Kramers–Kronig relation [Eq. (1)], and the delta function term gives the imaginary part.

Then, for the cumulant function, we first subtract the linear part and take the long-time limit to find

$$\begin{aligned}
\lim_{t\to\infty} \big[C^{\mathrm{R}}(t) + i\Sigma(\varepsilon)t\big] &= \int_{-\infty}^{\infty} \mathrm{d}\omega\, \beta(\omega+\varepsilon) \Big[\frac{e^{-i\omega t} - 1 + i\omega t}{\omega^2} + it\frac{e^{-i\omega t} - 1}{\omega}\Big] \\
&= \int_{-\infty}^{\infty} \mathrm{d}\omega\, \beta(\omega+\varepsilon) \frac{(1+i\omega t)e^{-i\omega t} - 1}{\omega^2} \\
&= -\int_{-\infty}^{\infty} \mathrm{d}\omega\, \beta(\omega+\varepsilon) \frac{\mathrm{d}}{\mathrm{d}\omega}\Big(\frac{e^{-i\omega t} - 1}{\omega}\Big)\,.
\end{aligned} \tag{A3}$$

Integrating by parts, we find

$$\begin{aligned}
\lim_{t\to\infty} \big[C^{\mathrm{R}}(t) + i\Sigma(\varepsilon)t\big] &= \int_{-\infty}^{\infty} \mathrm{d}\omega\, \frac{\mathrm{d}\beta(\omega+\varepsilon)}{\mathrm{d}\omega} \frac{e^{-i\omega t} - 1}{\omega} \\
&= \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \beta(\omega+\varepsilon) \frac{e^{-i\omega t} - 1}{\omega} = \frac{\mathrm{d}\Sigma(\omega)}{\mathrm{d}\omega}\bigg|_{\omega=\varepsilon}\,.
\end{aligned} \tag{A4}$$

This concludes the proof of Eq. (5).

[1] P.-F. Loos, A. Marie, and A. Ammar, Cumulant green's function methods for molecules (2024), arXiv:2402.16414 [physics.chem-ph].