

The Fourier transform of the quadratic Kubo-Bass term

The behavior given by the first two terms of the Kubo-Bass series is

$$B(t) = \int R(t')G_1(t-t')dt' + \int \int R(t')R(t'')G_2(t-t', t'-t'')dt'dt'' \quad . \quad (1)$$

While the Fourier transform of the linear term is well known, $r(f)g_1(f)$, the quadratic term has rarely been used. In the frequency domain the 2nd order term is given by

$$b_2(f) = \int e^{2\pi i f t} dt \int \int R(t')R(t'')G_2(t-t', t'-t'')dt'dt'' \quad . \quad (2)$$

Replacement of $R(t')$ and $R(t'')$ by their inverse Fourier transform representation[1] yields

$$\begin{aligned} b_2(f) &= \int e^{2\pi i f t} dt \int \int \left[\int r(f')e^{-2\pi i f' t'} df' \right] \left[\int r(f'')e^{-2\pi i f'' t''} df'' \right] G_2(t-t', t'-t'')dt'dt'' \quad , \quad (3) \\ &= \int dt \int dt' \int dt'' \int df' \int df'' e^{2\pi i(f t - f' t' - f'' t'')} G_2(t-t', t'-t'') r(f') r(f'') \quad . \quad (4) \end{aligned}$$

Set $v = t' - t''$ or $t'' = t' - v$ and $dt'' = -dv$, so that upon substitution and rearrangement of the integration order

$$\begin{aligned} b_2(f) &= - \int dt \int dt' \int df' \int df'' e^{2\pi i f t} \left[\int dv e^{-2\pi i(f' t' + f''(t' - v))} G_2(t-t', v) \right] r(f') r(f'') \quad , \quad (5) \\ &= - \int dt \int dt' \int df' \int df'' e^{2\pi i f t} \left[\int dv e^{-2\pi i(f' t' + f'' t' - f'' v)} G_2(t-t', v) \right] r(f') r(f'') \quad , \quad (6) \\ &= - \int dt \int dt' \int df' \int df'' e^{2\pi i f t} e^{-2\pi i(f' + f'')t'} \left[\int dv e^{2\pi i f'' v} G_2(t-t', v) \right] r(f') r(f'') \quad . \quad (7) \end{aligned}$$

Next set $u = t - t'$ or $t' = t - u$ and $dt' = -du$, hence upon substitution and further rearrangement

$$\begin{aligned} b_2(f) &= \int dt \int df' \int df'' \int du e^{2\pi i f t} e^{-2\pi i(f' + f'')(t-u)} \left[\int dv e^{2\pi i f'' v} G_2(u, v) \right] r(f') r(f'') \quad , \quad (8) \\ &= \int dt \int df' \int df'' \int du e^{2\pi i(f t - f' t + f' u - f'' t + f'' u)} \left[\int dv e^{2\pi i f'' v} G_2(u, v) \right] r(f') r(f'') \quad , \quad (9) \\ &= \int dt \int df' \int df'' \int du e^{2\pi i(f - f' - f'')t} e^{2\pi i(f' + f'')u} \left[\int dv e^{2\pi i f'' v} G_2(u, v) \right] r(f') r(f'') \quad , \quad (10) \\ &= \int df' \int df'' \int dt e^{2\pi i(f - f' - f'')t} \left[\int \int du dv e^{2\pi i(f' + f'')u} e^{2\pi i f'' v} G_2(u, v) \right] r(f') r(f'') \quad . \quad (11) \end{aligned}$$

The factor in the square parentheses is a two-dimensional Fourier transform, so Equation 11

can be rewritten in the simpler form of

$$b_2(f) = \int df' \int df'' \underbrace{\int dt e^{2\pi i(f-f'-f'')t}}_{\delta(f'' - (f-f'))} g_2(f' + f'', f'') r(f') r(f'') \quad . \quad (12)$$

Recognizing the bracketed factor in Equation 12 as the Fourier transform representation of $\delta((f - f') - f'')[2]$ and, that from symmetry it is also equal to $\delta(f'' - (f - f'))$, yields upon substitution and evaluation of the integral over df''

$$b_2(f) = \int df' \int df'' \delta(f'' - (f - f')) g_2(f' + f'', f'') r(f') r(f'') \quad , \quad (13)$$

$$= \int df' g_2(f' + (f - f'), f - f') r(f') r(f - f') \quad , \quad (14)$$

$$= \int df' g_2(f, f - f') r(f') r(f - f') \quad . \quad (15)$$

All that remains are the two small tasks of developing a stable numerical technique to estimate $g_2(f, f - f')$ from data and an experimental test of whether Equation 15 can outperform linear term.

References

- [1] Ron Bass both showed the value of replacing $R(t')$ and $R(t'')$ by their inverse Fourier transform representation and developed the general outline of this calculation in the early 1980's. This calculation is just a recovery of his original result.
- [2] Arfken, G. (1970). *Mathematical Methods for Physicists*, (pp. 671–673). New York:Academic Press.