Hilbert transform (NRG Ljubljana and TRIQS implementation)

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I. DEFINITION

The Hilbert transform of (spectral) function $A(\omega)$ is defined as

$$H(z) = \int_{-\infty}^{\infty} \frac{A(\omega)}{z-\omega} d\omega. \tag{1}$$

The argument is a complex number $z = x + iy$. For large $|y|$, this integral can be evaluated directly. The tabulated spectral function $A(\omega)$ is interpolated using cubic splines (GSL). Outside its domain of definition (tabulation range), the spectral function is taken to be equal to zero. The real and imaginary parts of the result are computed separately using real-valued integration:

$$\begin{aligned} \mathrm{Re}H(z) &= \int_{-\infty}^{\infty} \frac{\mathrm{Re}A(\omega)(x-\omega) + \mathrm{Im}A(\omega)y}{(x-\omega)^2+y^2} d\omega, \\ \mathrm{Im}H(z) &= \int_{-\infty}^{\infty} \frac{\mathrm{Re}A(\omega)(-y) + \mathrm{Im}A(\omega)(x-\omega)}{(x-\omega)^2+y^2} d\omega. \end{aligned} \tag{2}$$

We use 15-point Gauss-Kronrod rule (`GSL_INTEG_GAUSS15` argument to `gsl_integration_qag`). The accuracy goal is 10^{-14} absolute accuracy and 10^{-10} relative accuracy; failure to reach the goal is not considered an error and does not terminate the program.

For small $|y|$, we handle the singular point explicitly, by subtraction:

$$H(z) = \int_{-\infty}^{\infty} \frac{A(\omega)-A(x)}{z-\omega} d\omega + A(x) \int_{-\infty}^{\infty} \frac{1}{z-\omega} d\omega. \tag{3}$$

The second integral, $Q(z) = \int d\omega/(z-\omega)$, is evaluated analytically and expressed in terms of $\arctan$ and $\log$ functions. The first one is evaluated numerically after a change of variables, $\omega = x + |y|W$, $W = \exp(r)$ or $W = -\exp(r)$, with r ranging from $\log(10^{-16})$ to the boundary of the integration range, on both sides of the singularity. The ensures very high accuracy of the result.

II. INTERFACES

For scalar-valued $A(\omega)$, there are three interfaces:

- `hilbert_transform(A, z)` for single-point calculations,
- `hilbert_transform(A, mesh, eps = 1e-16)` for calculations on a mesh of real values with $y = \mathrm{eps}$, which produces the retarded Green's function on the real-frequency axis, (the corresponding advanced GF can be obtained using `eps = -1e-16`),
- `hilbert_transform(A, G)` for calculations on a set of complex values contained in a Green's function object $G(\omega)$, i.e., the output is $H[G(\omega)]$. This is useful in the context of DMFT where one needs to evaluate $H[\omega + \mu - \Sigma(\omega)]$.

For matrix-valued $A(\omega)$, there is an element-wise `hilbert_transform_elementwise` which threads over the matrix components.

For block GFs, there are two interfaces, one for single-point calculations and one for calculations one a mesh.