Fourier Transformations

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A. Direct Fourier Transformation

There are Fourier transformations, which are used in the program: direct ($\tau \rightarrow \omega$) and inverse one ($\omega \rightarrow \tau$). Because of only few points (maximum $L = 256$) we use cubic spline to get interpolation between those points and using known mathematical formula for the cubic spline and computed coefficients we take exactly Fourier integral. In the cubic spline we need to know coefficients in the interpolation formula:

$$G(\tau) = a_i + b_i(\tau - \tau_i) + c_i(\tau - \tau_i)^2 + d_i(\tau - \tau_i)^3$$

where $a_i = G(\tau_i)$, $b_i = G'(\tau_i)$, $c_i = G''(\tau_i)$, $d_i = G'''(\tau_i)$.
Or in terms of function, $G_i = G(\tau_i)$, and the second derivatives, $M_i = G''(\tau_i)$:

$$\begin{aligned} a_i &= G_i \\ b_i &= \frac{G_{i+1} - G_i}{h} - \frac{2M_i + M_{i+1}}{6}h \\ c_i &= \frac{M_i}{2} \\ d_i &= \frac{M_{i+1} - M_i}{6h} \end{aligned} \tag{1}$$

To obtain M_i coefficients we use the condition that the interpolated function is twice continuously differentiable on the interval . As the result we have $n+1$ equations for $n+3$ unknowns). we can get two additional equations from the boundary conditions. In the matrix form equations for M_i are the following:

$$\begin{bmatrix} 2 & \lambda_0 & & & & 0 \\ \mu_1 & 2 & \lambda_1 & & & \\ & \mu_2 & . & . & & \\ & & . & . & . & \\ & & . & . & 2 & \mu_{n-1} \\ 0 & & & & \mu_n & 2 \end{bmatrix} \begin{bmatrix} M_0 \\ M_1 \\ \cdots \\ \cdots \\ \\ M_n \end{bmatrix} = \begin{bmatrix} d_0 \\ d_1 \\ . \\ . \\ . \\ d_n \end{bmatrix} \tag{2}$$

where depending on boundary conditions a) when we know the first derivatives at the end points b) when we put the second derivatives at the end points equal to zero (natural spline) :

a)

$$\begin{aligned} \lambda_0 = 1,\ d_0 &= \frac{6}{h}\left(\frac{G_1 - G_0}{h} - G_0'\right) \\ \mu_0 = 1,\ d_n &= \frac{6}{h}\left(G_n' - \frac{G_n - G_{n-1}}{h}\right) \end{aligned}$$

b)

$$\lambda_0 = 0,\, d_0 = 0, \mu_0 = 0, d_0 = 0$$

and $\lambda_i = \mu_i = \frac{1}{2}$, for $i \in [1, n-1]$.

The second condition is not good enough for QMC computations especially for concentrations far from half-filling. More detailed derivations of the above formulae one can find in [1].

The first one is also difficult to fulfill because we do not know the first and the second derivatives at the end points, but what we know from physical properties of GF is the sum of the first and second derivatives at the end points, so called the first and the second moments of the GF. They are nothing else as the expansions of GF for high frequencies:

$$G(\omega) = \sum_{i=0}^{N} \frac{M^{(i)}}{\omega^{i+1}}, \tag{3}$$

where a momentum of k degree is defined as follows:

$$M^{(k)} = \int\limits_{-\infty}^{+\infty} d\omega \omega^k \rho(\omega), \tag{4}$$

where $\rho(\omega)$ is the Density of states (DOS).

Moments $M^{(k)}$ can be bind expressed sum of GFs and it's derivatives in imaginary-time space as:

$$G^{(k)}(0) + G^{(k)}(\beta) = M^{(k)}, \tag{5}$$

where $k = 0, \dots N$.

To show this one needs to take Fourier integral in parts:

$$\begin{aligned} G(i\omega_n) = & \sum_{k=0}^{N} \frac{(-1)^{k+1}(G^{(k)}(0) + G^{(k)}(\beta))}{(i\omega_n)^{k+1}} \\ & + \frac{(-1)^{N+1}}{(i\omega_n)^{N+1}} \int\limits_{0}^{\beta} \mathrm{e}^{i\omega_n \tau} \frac{\partial^{N+1} G(\tau)}{\partial \tau^{N+1}} d\tau. \end{aligned} \tag{6}$$

For N-degenerate Anderson model the first three moments moments obtained from corresponding commutators

$$M^{(k)} = \left\langle \{\mathcal{L}^k f_\sigma; f_\sigma^\dagger\}_+ \right\rangle,$$

where $\mathcal{L}^i \mathcal{O} = [\mathcal{O}, \mathcal{H}]$ is the commutator of operator $\mathcal{O}$ with the Hamiltonian, $\{...\}_+$ is the anticommutator, and for $SU(N)$ approximation read as

$$\begin{aligned} & M^{(0)} = 1, \\ & M^{(1)} = \langle \varepsilon + (2N-1)Un \rangle, \\ & M^{(2)} = \left\langle \varepsilon^2 + 2\varepsilon(2N-1)Un + (2N-1)U^2 \left[n + \tfrac{2C^2_{2N-1}}{2N-1} \langle nn \rangle \right] + \sum_k V^2_{k1} \right\rangle. \end{aligned} \tag{7}$$

If we know $M^{(i)}, i = 1,2,3$ we can rewrite the system of equations (2) and solve it. Below we give details how to do it.

$$\begin{array}{lllllll}
2M_0 & +\lambda_0 M_1 & & & & & = d_0 = \frac{6}{h}\left(\frac{\Delta y_1}{h} - y_0'\right) \\
\mu_1 M_0 & 2M & +\lambda_1 M_2 & & & & = d_1 = \frac{3}{h}\left(\frac{\Delta y_2}{h} - \frac{\Delta y_1}{h}\right) \\
 & \mu_2 M_1 & +2M_2 & +\lambda_2 M_3 & & & = d_2 \\
 & & \mu_3 M_2 & +2M_3 & +\lambda_3 M_4 & & = d_3 \\
 & & & \ddots & \ddots & \ddots & \vdots \\
 & & & \mu_{n-1} M_{n-2} & +2M_{n-1} & +\lambda_{n-1} M_n & = d_{n-1} \\
 & & & & \mu_n M_{n-1} & +2M_n & = d_n = \frac{6}{h}\left(y_n' - \frac{\Delta y_n}{h}\right)
\end{array}$$

$y_0' + y_n' = A;\ M_0 + M_n = B;\ \mu_n = \lambda_0 = 1;$ $\qquad$ $y_n' = A - y_0';\ M_n = B - M_0$

$$
\begin{array}{lllllll}
2M_0 & +\lambda_0 M & +\frac{6}{h}y_0' & & & & = \frac{6}{h}\frac{\Delta y_1}{h} \\
\mu_1 M_0 & 2M & +\lambda_1 M_2 & & & & = d_1 \\
 & \mu_2 M_1 & +2M_2 & +\lambda_2 M_3 & & & = d_2 \\
 & & \mu_3 M_2 & +2M_3 & +\lambda_3 M_4 & & = d_3 \\
 & & & \ddots & \ddots & \ddots & \vdots \\
-\lambda_{n-1} M_0 & & & \mu_{n-1} M_{n-2} & +2M_{n-1} & & = d_{n-1} - \lambda_{n-1} B \\
-2M_0 & & +\frac{6}{h}y_0' & & +\mu_n M_{n-1} & +2M_n & = d_n = \frac{6}{h}\left(A - \frac{\Delta y_n}{h}\right) - 2B
\end{array}
$$

$$\lambda_1 \to \lambda_{n-1} = \frac{1}{2};\ \mu_1 \to \mu_{n-1} = \frac{1}{2}$$

$$
\begin{array}{lllllll}
4M_0 & +M_1 & & & & -M_{n-1} & = d_0 = \frac{6}{h}\left(\frac{\Delta y_1}{h} + \frac{\Delta y_n}{h} - A\right) + 2B \\
\frac{1}{2}M_0 & +2M & +\frac{1}{2}M_2 & & & & = d_1 = \frac{3}{h}\left(\frac{y_2+y_0-2y_1}{h}\right) \\
 & \frac{1}{2}M_1 & +2M_2 & +\frac{1}{2}M_3 & & & = d_2 \\
 & & \frac{1}{2}M_2 & +2M_3 & +\frac{1}{2}M_4 & & = d_3 \\
 & & & \ddots & \ddots & \ddots & \vdots \\
 & & & \frac{1}{2}M_{n-3} & +2M_{n-2} & \frac{1}{2}M_{n-1} & = d_{n-2} = \frac{3}{h}\left(\frac{y_{n-1}+y_{n-3}-2y_{n-2}}{h}\right) \\
-\frac{1}{2}M_0 & & & & +\frac{1}{2}M_{n-2} & +2M_{n-1} & = d_{n-1} = \frac{6}{h}\left(\frac{y_n+y_{n-2}-2y_{n-1}}{h}\right) - \frac{1}{2}B
\end{array}
$$

$$
\begin{array}{llllll}
4M_0 & +M_1 & & & -M_{n-1} & = d_0 \\
 & q_1 M_1 & +\frac{1}{2}M_2 & & \frac{1}{2q_0}M_{n-1} & = d_1 - \frac{1}{2q_0}d_0 \\
 & \frac{1}{2}M_1 & +2M_2 & +\frac{1}{2}M_3 & & = d_2 \\
 & & \ddots & \ddots & \ddots & \vdots \\
 & \frac{1}{2q_0}M_1 & & +\frac{1}{2}M_{n-2} & +\left(2 - \frac{1}{2q_0}\right)M_{n-1} & = d_{n-1}^{(0)} + \frac{1}{2q_0}d_0
\end{array}
$$

$$
\begin{array}{llllll}
4M_0 & +M_1 & & & -M_{n-1} & = d_0 \\
 & q_1 M_1 & +\frac{1}{2}M_3 & & r_0 M_{n-1} & = \tilde{d}_1 \\
 & \frac{1}{2}M_1 & +2M_2 & +\frac{1}{2}M_3 & & = d_2 \\
 & & \ddots & \ddots & \ddots & \vdots \\
 & r_0 M_1 & & +\frac{1}{2}M_{n-2} & +p_1 M_{n-1} & = d_{n-1}^{(1)}
\end{array}
$$

$$
\begin{array}{llllll}
q_1 M_1 & +\frac{1}{2}M_2 & & & +r_0 M_{n-1} & = \tilde{d}_1 \\
 & q_2 M_2 & +\frac{1}{2}M_2 & & -\frac{1}{2q_1}r_0 M_{n-1} & = d_2 - \frac{1}{2q_1}\tilde{d}_1 \\
 & \frac{1}{2}M_2 & +2M_3 & +\frac{1}{2}M_4 & & = d_3 \\
 & & \ddots & \ddots & \ddots & \vdots \\
 & -\frac{r_0}{2q_1}M_2 & & +\frac{1}{2}M_{n-2} & +\left(p_1 - \frac{2r_0^2}{2q_1}\right)M_{n-1} & = d_{n-1}^{(1)} - \frac{r_0}{q_1}\tilde{d}_1
\end{array}
$$

$$
\begin{array}{llllll}
q_1 M_1 & +\frac{1}{2}M_2 & & & +r_0 M_{n-1} & = \tilde{d}_1 \\
 & q_2 M_2 & +\frac{1}{2}M_2 & & -r_1 M_{n-1} & = \tilde{d}_2 \\
 & \frac{1}{2}M_2 & +2M_3 & +\frac{1}{2}M_4 & & = d_3 \\
 & & \ddots & \ddots & \ddots & \vdots \\
 & -r_1 M_2 & & +\frac{1}{2}M_{n-2} & +p_2 M_{n-1} & = d_{n-1}^{(2)}
\end{array}
$$

$$\begin{array}{llllll}
q_2 M_2 & +\frac{1}{2}M_3 & & & -r_1 M_{n-1} & = \tilde{d}_2 \\
 & q_3 M_3 & +\frac{1}{2}M_4 & & +\frac{r_1}{2q_2}M_{n-1} & = d_3 - \frac{1}{2q_2}\tilde{d}_2 \\
 & \frac{1}{2}M_3 & +2M_4 & +\frac{1}{2}M_5 & & = d_4 \\
 & & \ddots & \ddots & \ddots & \vdots \\
 & \frac{r_1}{2q_2}M_3 & & +\frac{1}{2}M_{n-2} & +\left(p_2 - \frac{r_1 r_1}{q_2}\right)M_{n-1} & = d^{(2)}_{n-1} + \frac{r_1}{q_2}\tilde{d}_2
\end{array}$$

$$\begin{array}{llllll}
q_3 M_3 & +\frac{1}{2}M_4 & & & +r_2 M_{n-1} & = \tilde{d}_3 \\
\frac{1}{2}M_3 & +2M_4 & +\frac{1}{2}M_5 & & & = d_4 \\
 & \ddots & \ddots & \ddots & \vdots & \\
r_2 M_3 & & +\frac{1}{2}M_{n-2} & +p_3 M_{n-1} & & = d^{(3)}_{n-1}
\end{array}$$

Some Definitions

$$\begin{array}{llll}
q_0 = 4 & \tilde{d}_0 = d_0 & p_0 = 2 & \\
r_0 = \frac{1}{2q_0} & \tilde{d}_1 = d_1 - \frac{1}{2q_0}d_0 & p_1 = 2 - \frac{1}{2q_0} = 2 - r_0 & d^{(1)}_{n-1} = d_{n-1} + \frac{d_0}{2q_0} \\
r_1 = \frac{1}{2q_1}r_0 & \tilde{d}_2 = d_2 - \frac{1}{2q_1}\tilde{d}_1 & p_2 = p_1 - 2r_1 r_0 & d^{(2)}_{n-1} = d^{(1)}_{n-1} - 2r_1\tilde{d}_1 \\
r_2 = \frac{1}{2q_2}r_1 & \tilde{d}_3 = d_3 - \frac{1}{2q_2}\tilde{d}_2 & p_3 = p_2 - 2r_2 r_1 & d^{(3)}_{n-1} = d^{(2)}_{n-1} + 2r_2\tilde{d}_2
\end{array} \tag{8}$$

$$r_k = \frac{1}{2q_k}r_{k-1};\;\; q_k = 2 - \frac{1}{2}\frac{1}{2q_{k-1}},\; k \geq 2;\; q_1 = 2 - \frac{1}{2q_0};$$

$$d_i = \frac{6}{h}\left(\frac{y_{i+1} + y_{i-1} - 2y_i}{h}\right);\;\; d_0 = \frac{6}{h}\left(\frac{\Delta y_1 + \Delta y_n}{h} - A\right) + 2B;\;\; d_{n-1} = \frac{6}{h}\left(y_n + y_{n-2} - 2y_{n-1}\right) - \frac{1}{2}B;$$

$$\begin{array}{llllll}
q_{n-5}M_{n-5} & +\frac{1}{2}M_{n-4} & & & +r_{n-6}M_{n-1} & = \tilde{d}_{n-5} \\
\frac{1}{2}M_{n-5} & +2M_{n-4} & +\frac{1}{2}M_{n-3} & & & = d_{n-4} \\
 & \frac{1}{2}M_{n-4} & +2M_{n-3} & +\frac{1}{2}M_{n-2} & & = d_{n-3} \\
 & & +\frac{1}{2}M_{n-3} & +2M_{n-2} & +\frac{1}{2}M_{n-1} & = d_{n-2} \\
r_{n-6}M_{n-5} & & & +\frac{1}{2}M_{n-2} & +p_{n-5}M_{n-1} & = d^{(n-5)}_{n-1}
\end{array}$$

$$\begin{array}{llllll}
q_{n-4}M_{n-4} & +\frac{1}{2}M_{n-3} & & & -r_{n-5}M_{n-1} & = \tilde{d}_{n-4} \\
\frac{1}{2}M_{n-4} & +2M_{n-3} & +\frac{1}{2}M_{n-2} & & & = d_{n-3} \\
 & \frac{1}{2}M_{n-3} & +2M_{n-2} & +\frac{1}{2}M_{n-1} & & = d_{n-2} \\
 & & +\frac{1}{2}M_{n-3} & +2M_{n-2} & +\frac{1}{2}M_{n-1} & = d_{n-2} \\
-r_{n-5}M_{n-4} & & & +\frac{1}{2}M_{n-2} & +p_{n-4}M_{n-1} & = d^{(n-4)}_{n-1}
\end{array}$$

$$\begin{array}{llll}
q_{n-3}M_{n-3} & +\frac{1}{2}M_{n-2} & r_{n-4}M_{n-1} & = \tilde{d}_{n-3} \\
+\frac{1}{2}M_{n-3} & +2M_{n-2} & +\frac{1}{2}M_{n-1} & = d_{n-2} \\
r_{n-4}M_{n-3} & +\frac{1}{2}M_{n-2} & +p_{n-3}M_{n-1} & = d^{(n-3)}_{n-1}
\end{array}$$

$$\left\{\begin{array}{llll}
q_{n-2}M_{n-2} & & +\left(\frac{1}{2} - r_{n-3}\right)M_{n-1} & = \tilde{d}_{n-2} \\
\left(\frac{1}{2} - r_{n-3}\right)M_{n-2} & +p_{n-2}M_{n-1} & & = d^{(n-2)}_{n-1}
\end{array}\right.$$

$$\left(p_{n-2} - \frac{\left(\frac{1}{2} - r_{n-3}\right)^2}{q_{n-2}}\right)M_{n-1} = d^{(n-2)}_{n-1} - \frac{\left(\frac{1}{2} - r_{n-3}\right)}{q_{n-2}}\tilde{d}_{n-2} \rightarrow$$

$$M_{n-1} = \frac{d_{n-1}^{(n-2)} - \frac{\left(\frac{1}{2} - r_{n-3}\right)}{q_{n-2}}\tilde{d}_{n-2}}{p_{n-2} - \left(\frac{1}{2} - r_{n-3}\right) M_{n-1}},$$

$$M_{n-2} = \frac{\tilde{d}_{n-2} - \left(\frac{1}{2} - r_{n-3}\right)}{q_{n-2}} M_{n-1},$$

$$M_k = \frac{\tilde{d}_k + (-1)^k r_{k-1} M_{n-1} - \frac{1}{2} M_{k+1}}{q_k}.$$

Now having obtained second derivatives M_i and coefficients a_i, b_i, c_i, d_i we can take Fourier integral analytically. It was done using Mathematica. Printout from Mathematica presented below (pay attention that in Mathematica we used slightly different notations):

$$F[i] = Integrate[\quad (a - b*(t - d*i) + c*(t - d*i)^2 - e*(t - d*i)^3)*\exp[I*t*w], \{t, d*(i-1), d*i\}] =$$

$$\frac{\exp^{I*d*i*w}*(-6*e + 2*I*c*w + b*w^2 - I*a*w^3)}{w^4} - \tag{9}$$

$$\frac{1}{w^4}(\exp^{I*d*(-1+i)*w}*(-6*e + 2*I*c*w - 6*I*d*e*w + b*w^2 - 2*c*d*w^2 +$$

$$3*d^2*e*w^2 - I*a*w^3 + I*b*d*w^3 - I*c*d^2*w^3 + I*d^3*e*w^3))$$

Sum over i of $F(i)$ will give us the Fourier integral in frequency space. This formula can be very easily identified in the corresponding subroutine.

B. Inverse Fourier Transformation

Green function $G(\omega)$ falls off as $1/\omega$ when $\omega \to \infty$. In the program we deal with finite number of frequency points and cutting $1/\omega$ tail is the crude approximation. By cutting off this tail, the discontinuity of GF $G(\tau)$ is removed. In this case, the high-frequency tail has to be extracted and Fourier transformed analytically, by using the Fourier relation

$$\frac{1}{i\omega_n - \epsilon} \leftrightarrow -[\Theta(\tau) + \zeta n(\epsilon)]\, e^{-\epsilon\tau}, \tag{10}$$

where $n(\epsilon) \equiv 1/[\exp\{\beta\epsilon\} - \zeta]$ and $\zeta = \pm 1$ depending on whether ω_n is bosonic or fermionic.

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[1] J. Stoer, and R. Bulirsch, '*Introduction to Numerical Analysis*',Springer-Verlag NY, 1980.