make the evaluation of the corresponding self-consistency equations pointless. In particular, in the naive scheme, the self-energy diverges near the Nyquist frequency. Finally, the sum in (3.15) is numerically somewhat unstable since $\widetilde{G}(\tau)$ also oscillates between the grid points τ_l.

Splining Method

Fortunately, there is physical information left that has not been used in the naive scheme: $G(\tau)$ is known to be a smooth function. In fact, it follows from (1.55) and (1.56) that $G(\tau)$ and all even derivatives are positive definite and, consequently, reach their maxima at the edges $\tau = 0$ and $\tau = \beta$. This knowledge of "smoothness" can be exploited in a spline interpolation of the QMC result $\{G(\tau_l)\}_{l=0}^{\Lambda}$ by piecewise cubic polynomials. The resulting functions may then either be used for oversampling, i.e., for generating $G(\tau)$ on a finite grid or for piecewise direct analytic Fourier transforms. In both cases, $G(i\omega_n)$ can be calculated for a much larger frequency range than before. Jarrell, Akhlaghpour, and Pruschke (1993) used oversampling with typically 800 Matsubara frequencies. The second choice mentioned above is implemented in Krauth's program: for any choice of Λ, $G(i\omega_n)$ is evaluated for a very large number (by default $N = 2^{13} = 8192$) of Matsubara frequencies. While the spline interpolation incorporates some physical information, it is clearly not exact; therefore, the method used on its own has its limits. Jarrell noted that the usual cubic splines with continuous second derivative were dangerous in this respect since they tend to generate artificial high-frequency features. This effect was found to be reduced using Akima splines. Both implementations use splines with natural boundary conditions, i.e., with vanishing second derivative at the end points.

As we noted recently, this is in general not a good choice; after all, the true second derivatives are maximal at the end points. The bad fit at the boundaries then leads to ringing (which decays faster for Akima splines). An implementation with free boundary conditions for the second derivative which are determined in an iterative minimalization scheme was found to be vastly superior over both schemes at least for a restricted set of test cases. The minimization procedure can even be avoided by computing the second derivative of $G(\tau)$ at $\tau = 0$ exactly. A related method for improving on the natural spline scheme is to interpolate not $\{G(\tau_l)\}_{l=0}^{\Lambda}$, but only the difference with respect to some reference Green function obtained from, e.g., plain second order perturbation theory or IPT. This approach, discussed in a general context by Deisz, Hess, and Serene (1995), is implemented in Jarrell's code. In addition, the high-frequency part may be directly stabilized by supplementing the QMC estimates with IPT (using low-pass/high-pass filters). Since each of the approaches discussed so far generates a number of Matsubara frequencies which is much greater than the number of time slices, the inverse Fourier transform is unproblematic: the rounding-off near $\tau = 0$ is already small for the first grid point $\tau = \Delta\tau$ while at the end points $\tau = 0$ and $\tau = \beta$, the numerical Fourier transforms can be shifted by the value 1/2 to exactly cancel the rounding effect. For more information on recent developments, see App. C and Knecht's (2002) diploma thesis.