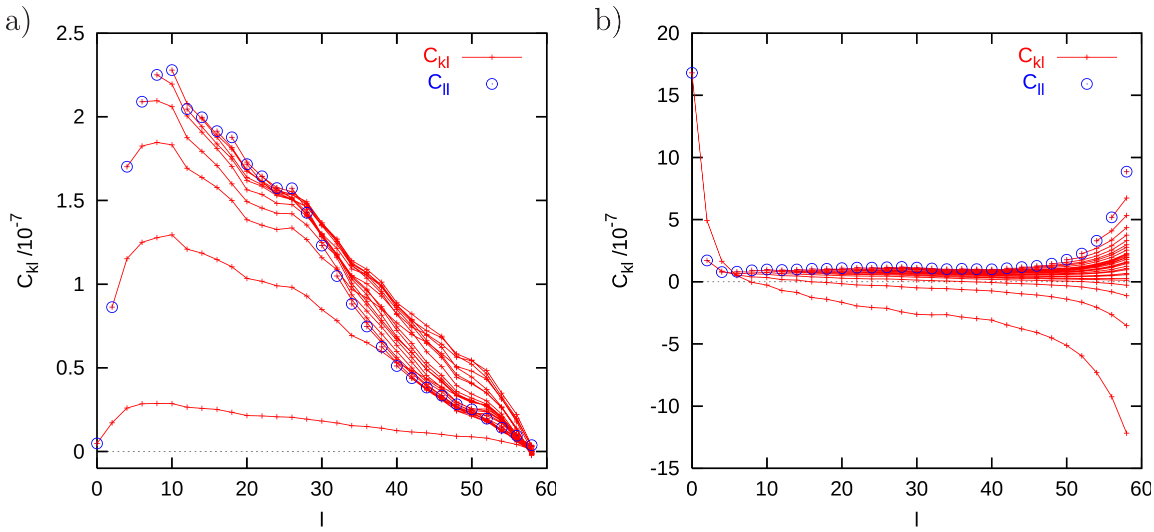

Figure 3.68: Covariance matrix C_{kl} of the 3-band QMC estimate of $G(\tau)$ for (asymmetric) LDA DOS of $La_{1-x}Sr_xTiO_3$, $n = 0.94$, $T = 1/10$, $U = 5.0$, and $\Delta\tau = 0.167$ (i.e., $\Lambda = 60$) using 102 measurements with 100000 sweeps each. The indices extend over $0 \le k \le l \le \Lambda - 1$; the missing elements follow from the symmetry $C_{kl} = C_{lk}$ and the constraint $G(0)+G(\beta) = 1$. **a)** Covariance matrix computed from band-averaged QMC measurements of G. **b)** Covariance matrix computed from QMC measurements of G for individual bands.

when χ^2 is generalized as

$$\chi^2 = \sum_{k,l=1}^{\Lambda} \left(\bar{G}_k - G_k\right) [C^{-1}]_{kl} \left(\bar{G}_l - G_l\right) . \tag{3.67}$$

In practice, it is necessary to apply a singular value decomposition (SVD) for diagonalizing the matrix C for repeated use in the computation and to work with rotated data $\bar{G}'_l$ and σ'_l. A SVD of the kernel K can also greatly accelerate the search for a solution. Another improvement realized in advanced codes is the possibility of marginalizing the spectrum over the Lagrange parameter α ("Bryan's method"). Jarrell's (1997) program [primarily based on Bryan (1990) and Gubernatis et al. (1991)] also used in this work realizes all of the improvements mentioned in this paragraph and also allows for a nonuniform frequency grid. While it yields more reliable spectra than the Sandvik code and even computes error bars for the integrated spectral weight in some finite regions, it requires more data sets and some additional efforts in order to produce stable results.

Non-Gaussian Error Distribution

One problem which arises both for the Sandvik and the Jarrell code is that the assumption of a Gaussian distribution of errors breaks down for $G(\tau)$ with $\tau \approx \beta/2$ in gapped systems at low temperatures T. This is illustrated by the histogram of measurements of $G(\beta/2)$ for the Bethe DOS, $T = 1/20$, and $U = 5.0$ shown in