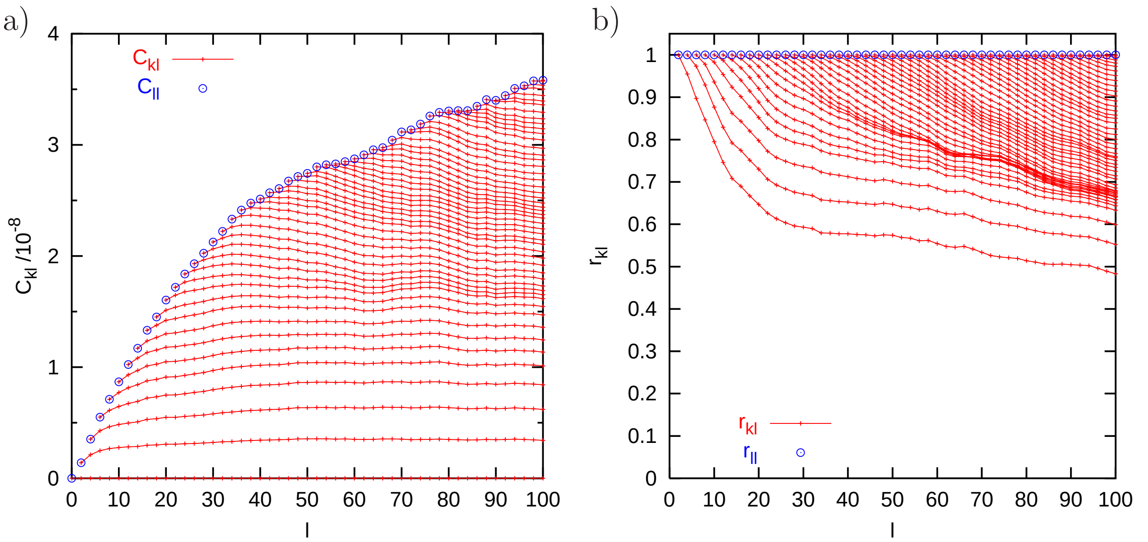


**Figure 3.67: a)** Covariance matrix $C_{kl}$ of the QMC estimate of $G(\tau)$ for Bethe DOS, $T = 1/20$, $U = 4.6$, and $\Delta\tau = 0.1$ (i.e., $\Lambda = 200$) using 300 bins with 10000 sweeps each. Circles indicate diagonal elements $C_{ll}$ as a function of $j$; offdiagonal elements with the same value of $k$ (crosses) are connected by a solid line. The indices extend over $0 \leq k \leq l \leq \Lambda/2$ (and correspond to $\tau_k = k\Delta\tau$, $\tau_l = l\Delta\tau$); the missing elements follow from the symmetries $C_{kl} = C_{lk}$ and (here) $G(\tau) = G(\beta - \tau)$. **b)** Corresponding Pearson's coefficients $r_{kl}$. For enhanced clarity, only even indices are included in the plots.

elements are additionally denoted by circles. Evidently, the offdiagonal elements are generically of the same order of magnitude as the diagonal elements. This shows that QMC measurements of the imaginary-time Green function $G$ at different time slices $\tau_l$ are not independent, but are instead highly correlated; in Bryan's terminology the full data set is oversampled. The same data is shown in a different representation in Fig. 3.67 b; here, each column and each row has been divided by the square root of the corresponding diagonal element. The result is a matrix of Pearson's coefficients $r_{kl}$, a dimensionless measure of linear correlation between pairs of stochastic variables.

Corresponding plots of the covariance matrix for an asymmetric case (LDA DOS of $La_{1-x}Sr_xTiO_3$ , $n = 0.94$, $T = 1/10$, and $U = 5.0$) are shown in Fig. 3.68. Since all three bands are degenerate and since measurements of $G$ for each band are highly correlated (e.g., the occupancy of individual bands fluctuates while the total occupancy is almost exactly constant), the most relevant covariance matrix for this case is that shown in Fig. 3.68 a for the band-averaged case; Fig. 3.68 b which applies to measurements of $G$ for one individual band (with much larger variances for $\tau \to 0$ and $\tau \to \beta$) is included for comparison and for later discussion in chapter 5 (in subsection 5.4.2). All results clearly demonstrate the large degree of covariance present in QMC estimates of $G(\tau)$.

Thus, a more general formulation of the MEM should be used which takes into account all elements of the covariance matrix. In principle, this is simple since the form (1.65) of the probability function still applies (in the limit of large bin size)