perfect. In particular, the curves for $U_c(T)$ are on top of each other for $T \geq 0.025$. The discrepancy for lower temperatures is also small; still, it exceeds the uncertainty of our results. This is illustrated in the inset of Fig. 3.52 where our original estimate of October 2000 is also shown. Even though the inclusion of additional QMC simulations and a refinement of the extrapolation and fitting methods have shifted our estimates of the extent of the coexistence region and of the position of the critical point considerably, the old and new estimate of $U_c(T)$ agree within linewidths in the low-temperature range. In comparison, Tong et al.'s (2001) result deviates markedly.

The excellent overall agreement between both sets of results shown in Fig. 3.52 is even more surprising in view of the fact that the methodology employed by Tong et al. (2001) is not exact. It is based on the replacement of the original DMFT problem by a modified set of self-consistency equations. In order to obtain a result for some interaction U, an impurity problem is solved for some different interaction U'. Up to a constant offset, the shift $U' - U$ is taken proportional to the midpoint-value of the imaginary-time Green function $G(\beta/2)$ which is here regarded as order parameter (which implies a self-consistency condition for U'). Since the absolute value of the order parameter is larger within the metallic phase throughout the coexistence region (with decreasing difference towards the critical end point), the overlap in terms of U' can be reduced until it vanishes by choosing the proportionality constant sufficiently large. The solutions of the modified self-consistency problem then becomes not only unique in terms of U', but a new solution appears which continuously spans the gap in terms of U' between the solutions associated with the coexisting solutions of the original problem. For the modified problem, all observables are smooth functions of U'. When folding back the results into the original parameter space (i.e., by plotting the results in terms of U rather than U'), the additional solution is interpreted as a third, thermodynamically unstable, phase; observables measured for the modified problem appear as smooth s-shaped curves. This is seen in in Fig. 3.53, where full symbols represent Tong et al.'s (2001) results for the double occupancy. Apart from the square-root singularity of the metallic solution at U_{c2} suggested by this method and from the additional unstable solution, the main difference in comparison to our QMC results is a shift towards larger values of D. This discrepancy is highly significant deep in the insulating phase (say: for $U \geq 5.6$) where the error of the QMC results is of the order 10^{-4}, i.e., within linewidth. At the ground state transition point $U_c^0 \approx 5.85$, Tong et al. predict $D \approx 0.02$ which is far above our estimate $D \approx 0.0161$ and the PSCT result $D \approx 0.015$. Furthermore, the temperature dependence in this region is several orders of magnitude too large and is of the wrong sign. This observation already points to the main problem of the method: it cannot be exact since the impurity model is in general solved at a shifted interaction U' instead of U. As noted in Sec. 4.6, the second moment of the self-energy is independent of the hybridization and only depends on the interaction on the impurity, equaling $U^2/4$. For the Bethe DOS, this second moment also determines the second derivative of $G(\tau)$ at $\tau = 0$. Consequently, the measurements of $G(\tau)$ performed by Tong et al. must suffer from systematic errors due to shifting the interaction, regardless of details of the self-consistency scheme (which influences the hybridization function). Still, the high accuracy of the final results cannot be accidental. In our view, the qualitative