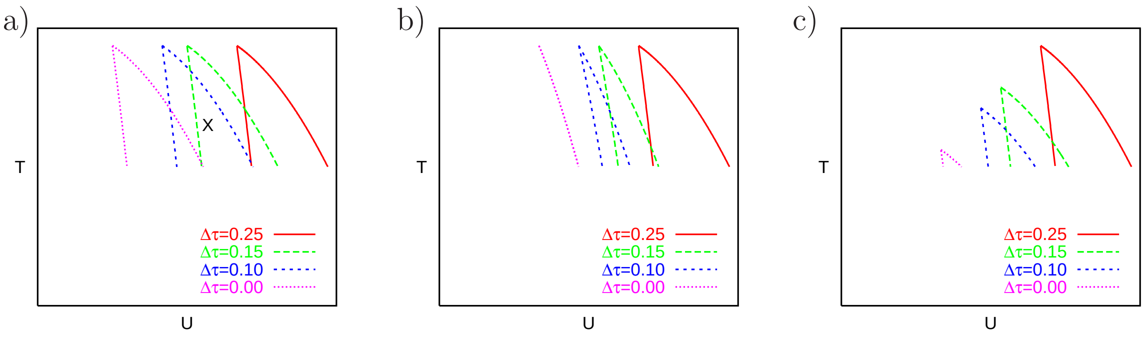

Figure 3.13: Scenarios for the effect of a $\Delta\tau \to 0$ extrapolation on the coexistence region: **a)** coexistence region shifts to smaller U at constant shape, **b)** coexistence region shrinks with constant critical temperature T^*, **c)** coexistence region shifts to smaller U and T, i.e., shrinks within the attainable temperature range.

3.4.2 Overrelaxation and Sweeping Strategies

One point that we have not discussed so far is the dependence of the shape and extent of the coexistence region on the discretization variable $\Delta\tau$. It is important to remember that the numerical results are only physically relevant after an extrapolation to $\Delta\tau = 0$. While Rozenberg et al.'s (1999) results for $\Delta\tau \geq 0.25$ make it likely that the observed coexistence persists at $\Delta\tau = 0$, both the remaining errors in the Fourier transformation and the inevitable Trotter error could have influenced the phase diagram considerably. Using the knowledge that U_{c2} decreases with decreasing $\Delta\tau$ [this is already apparent from Schlipf's (1998) results], the scenarios depicted schematically in Fig. 3.13 appear possible: If the coexistence region is merely shifted to lower U at roughly constant shape (Fig. 3.13 a), the conclusions drawn from $\Delta\tau = 0.25$ may be regarded as essentially correct. If, in contrast, the coexistence region shrunk with decreasing $\Delta\tau$ and vanished for $\Delta\tau = 0$ (Fig. 3.13 b), the picture at finite $\Delta\tau$ would be qualitatively incorrect. The existence of a first-order transition would then appear as an artifact for finite $\Delta\tau$. As an intermediate case, the coexistence region could also shrink with the critical temperature T^* being considerably reduced for $\Delta\tau \to 0$. Then, the conclusions from $\Delta\tau = 0.25$ would still be qualitatively correct for the full phase diagram, but not for the temperature region under consideration. In subsection 3.5.4, will show that the $\Delta\tau \to 0$ extrapolation corresponds in leading order to a shift to smaller U, but also to slightly smaller T which is somewhere in between the scenarios Fig. 3.13 a and Fig. 3.13 c.

Still, the question remains why Jarrell did not see the small coexistence region for $T = 1/30$ in his contribution to our paper (Schlipf et al., 1999). The answer includes two aspects. Both are related to methods that usually improve the convergence process of DMFT simulations both in speed and in quality, but may fail to detect multiple solutions. The first method essentially incorporates an extrapolation to small $\Delta\tau$ within the iteration process: starting with relatively large $\Delta\tau$, some iterations are performed; then, $\Delta\tau$ is decreased before continuing the iteration process. Thus, costly iterations at small $\Delta\tau$ are usually only performed when the input