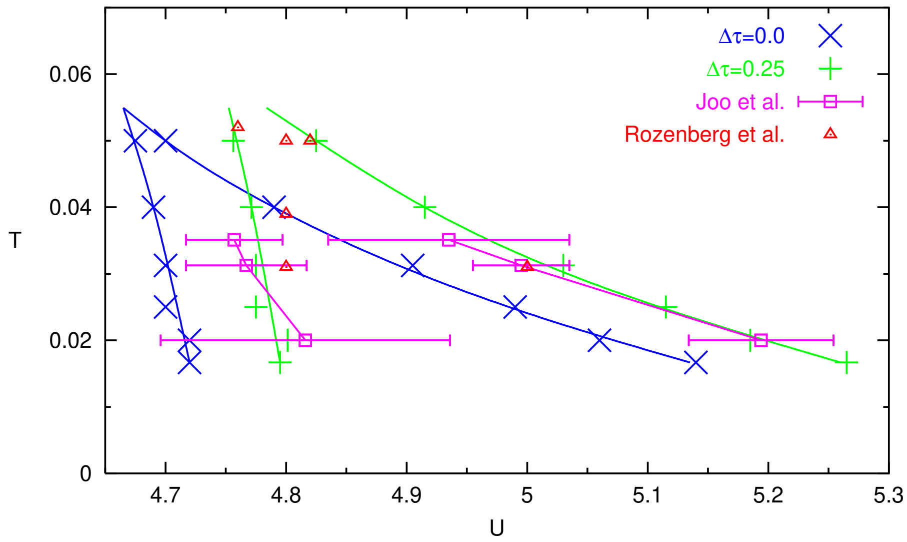

Figure 3.33: MIT phase diagram: dependency of the boundaries $U_{c1}(T)$ and $U_{c2}(T)$ of the coexistence region on $\Delta\tau$. Final results of this work for $\Delta\tau = 0.0$ (already shown in Fig. 3.31) and $\Delta\tau = 0.25$ in comparison with Joo and Oudovenko's (2001) results and the coexistence points established by Rozenberg et al. (1999).

the coexistence region which appear *a priori* possible, the scenario of Fig. 3.13 a is realized: finite $\Delta\tau$ primarily shifts the coexistence region towards larger values of U. Consequently, the coexistence found by Rozenberg can now *a posteriori* be assessed as genuine (and not as an artifact of using finite $\Delta\tau$).

Another fact established by these recent studies is that U_{c1} is almost independent of T, only slightly increasing when the temperature is lowered from $T = T^*$ to $T = 0$. This finding is clearly incompatible with the MIT scenario Fig. 3.10 suggested by Kotliar which partially reconciled QMC results (at relatively high temperature) with (zero-temperature) RDA results by assuming that $U_{c1}(T = 0) = 4.0$. Ironically, our correction of this perception of the shape of the coexistence region validates *a posteriori* the qualitative features of the IPT scenario (cf. Fig. 3.7 and Fig. 3.32), originally supported by Kotliar (and others).

3.5.5 Double Occupancy

In this subsection, we construct an extrapolation scheme for the double occupancy D in the metallic phase. In connection with the expression (3.19) established for the double occupancy of the insulating phase in subsection 3.5.1, the resulting estimates will allow for a determination of the difference $\Delta D(T, U)$ in double occupancy between metal and insulator within a few percent. This data will be used in combination with corresponding estimates energetic differences $\Delta E(T, U)$ (obtained in subsection 3.5.3) for the construction of a differential equation governing the thermodynamic first-order phase transition line $U_c(T)$ in Sec. 3.6. In addition to our best