which is equivalent to

$$\frac{\mathrm{d}U_\mathrm{c}(\beta)}{\mathrm{d}\beta} = -\frac{\Delta E(\beta, U_\mathrm{c}(\beta))}{\beta \Delta D(\beta, U_\mathrm{c}(\beta))} \tag{3.28}$$

$$= \frac{1}{\beta}\left(-\frac{\Delta E_\mathrm{kin}(\beta, U_\mathrm{c}(\beta))}{\Delta D(\beta, U_\mathrm{c}(\beta))} - U_\mathrm{c}\right). \tag{3.29}$$

While the second form (3.29) is somewhat more elementary, it conveys the wrong impression that large errors should be expected due to the subtraction of numbers of the same order of magnitude. This problem does not occur here since the numerical error of E is significantly smaller (by about a factor of two or three) than the error of E_kin. Therefore, we will in the following proceed with the total energy, i.e., use (3.28). Changing variables from β to T we arrive at the final form of the differential equation:[37]

$$\boxed{\frac{\mathrm{d}U_\mathrm{c}(T)}{\mathrm{d}T} = f(T, U_\mathrm{c}(T)); \qquad f(T,U) := \frac{\Delta E(T,U)}{T\,\Delta D(T,U)}.} \tag{3.30}$$

Since $U_\mathrm{c}(T)$ has to go through the tip of the coexistence region ($T = T^*$) where $U_{\mathrm{c}1} = U_{\mathrm{c}2} = U^*$, the true phase transition line $U_\mathrm{c}(T)$ is uniquely defined as the solution of (3.30) satisfying the initial condition $U_\mathrm{c}(T^*) = U^*$:

$$U_\mathrm{c}(T) = U^* + \int_{T^*}^{T} \mathrm{d}T' f(T', U_\mathrm{c}(T')); \quad T < T^*. \tag{3.31}$$

The slope of this curve is negative everywhere as we can see from the following argument: In going from an insulator to a metal, the entropy decreases. In order for the free energies to coincide at $U = U_\mathrm{c}(T)$, the change in total energy $\Delta E(T,U)$ has to be negative. Since the double occupancy increases at the same time, (3.30) yields $\mathrm{d}U_\mathrm{c}(T)/\mathrm{d}T < 0$.

In principle, $f(T,U)$ can be evaluated pointwise at finite $\Delta\tau$ by calculating the differences of D and U for fixed U and T. This was, in fact, our initial approach.[38] It is, however, not applicable near the edges and in the tip of the coexistence region, since the phase boundaries shift significantly with changing $\Delta\tau$. Consequently, in general, not enough (if any) data points are available for an extrapolation $\Delta\tau \to 0$ at fixed U.[39] Furthermore, an interpolation between the grid points (in U and T) at some stage is unavoidable in order to integrate up the formal solution (3.31).

[37] Note that this differential equation is in direct analogy to the Clausius-Clapeyron equation $\mathrm{d}p/\mathrm{d}T = \Delta Q/(T\Delta V)$ for the vapor pressure curve $p(T)$, where ΔQ is the latent heat and ΔV the volume difference between the two phases.

[38] This strategy yields accurate results deep within the coexistence region, where the resulting estimates for $f(T,U)$ are easily extrapolated to $\Delta\tau = 0$. The nearly linear dependence of $f(T,U)$ on U observed using this method motivated the linearization of the differential equation which we will introduce below.

[39] The difficulties associated with an extrapolation of D_m to $\Delta\tau = 0$ at fixed U clearly add to the problem (cf. subsection 3.5.5)