232U Spacing Comparison

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For this test, I varied the grid spacing in both Q_{20} and Q_{30}, using Dijkstra's algorithm. The different grids were obtained using a cubic spline interpolator of the actual PES. The final endpoint was selected, by Dijkstra's algorithm, to be the minimal action value from the ground state. All tests were done without the inertia tensor.

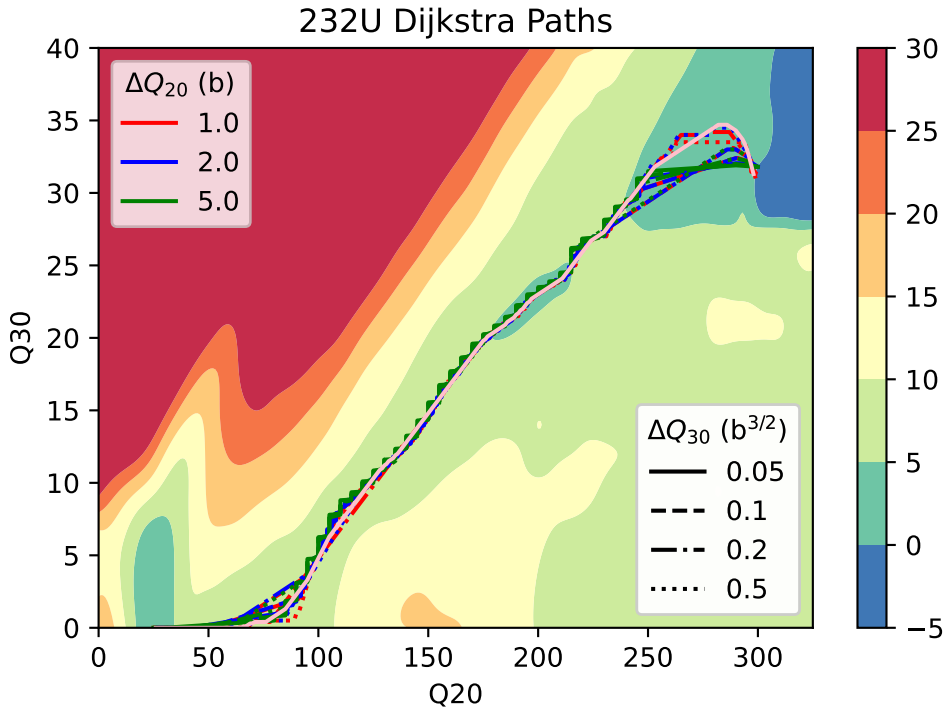

Figure 1: The above shows all of the paths. As can be seen there is quite a bit of variance. Sylvester's path is shown in pink; it is close to paths with a grid spacing of $\Delta Q_{20} = 1$, 2 and $\Delta Q_{30} = 0.5$, but does not agree with either.

Spacing	1.0	2.0	5.0	10.0
0.050	963.600	1040.200	1090.700	1095
0.100	952.100	1019.100	1077.900	1107.100
0.200	913.600	976.200	1064.700	1095
0.500	928.800	915.700	997.300	1054.700

Table 1: Action values for different spacings. All actions computed by interpolating the paths and using 500 points along the path. For comparison, Sylvester's code (with a spacing of $(1, 0.1)$) gives an action value of 909.810 using the same methodology. Different columns are Q_{20} spacings, in b; different rows are Q_{30} spacings, in $b^{3/2}$.

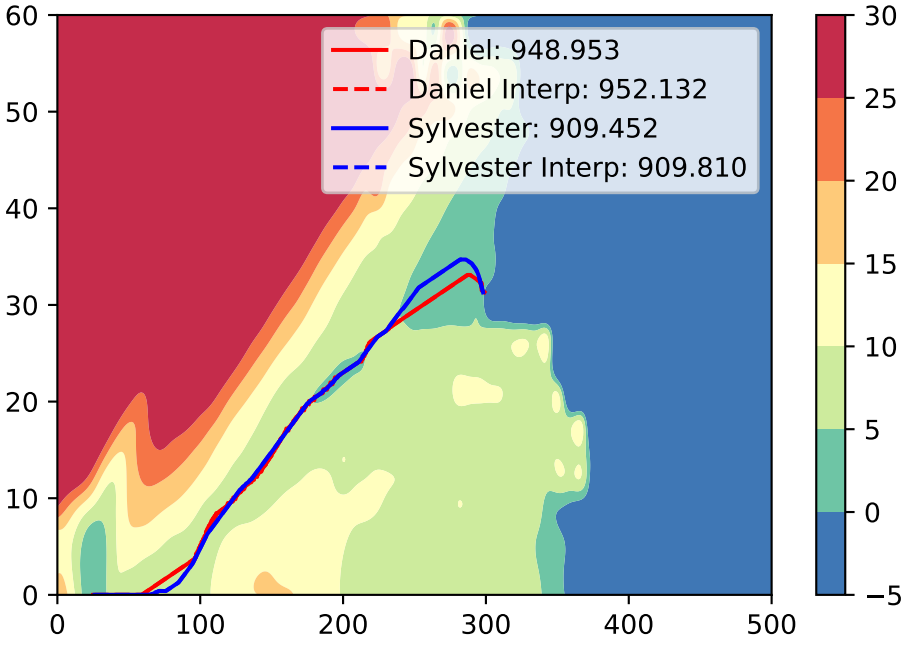

Figure 2: The above shows my path and Sylvester's path for the same grid spacing. As can be seen, they disagree noticeably, and indeed have quite different action values.