

**Sampling initial positions and momenta
for nuclear trajectories
from quantum mechanical distributions.**

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Supplementary Material.

S1 Pure Wigner sampling

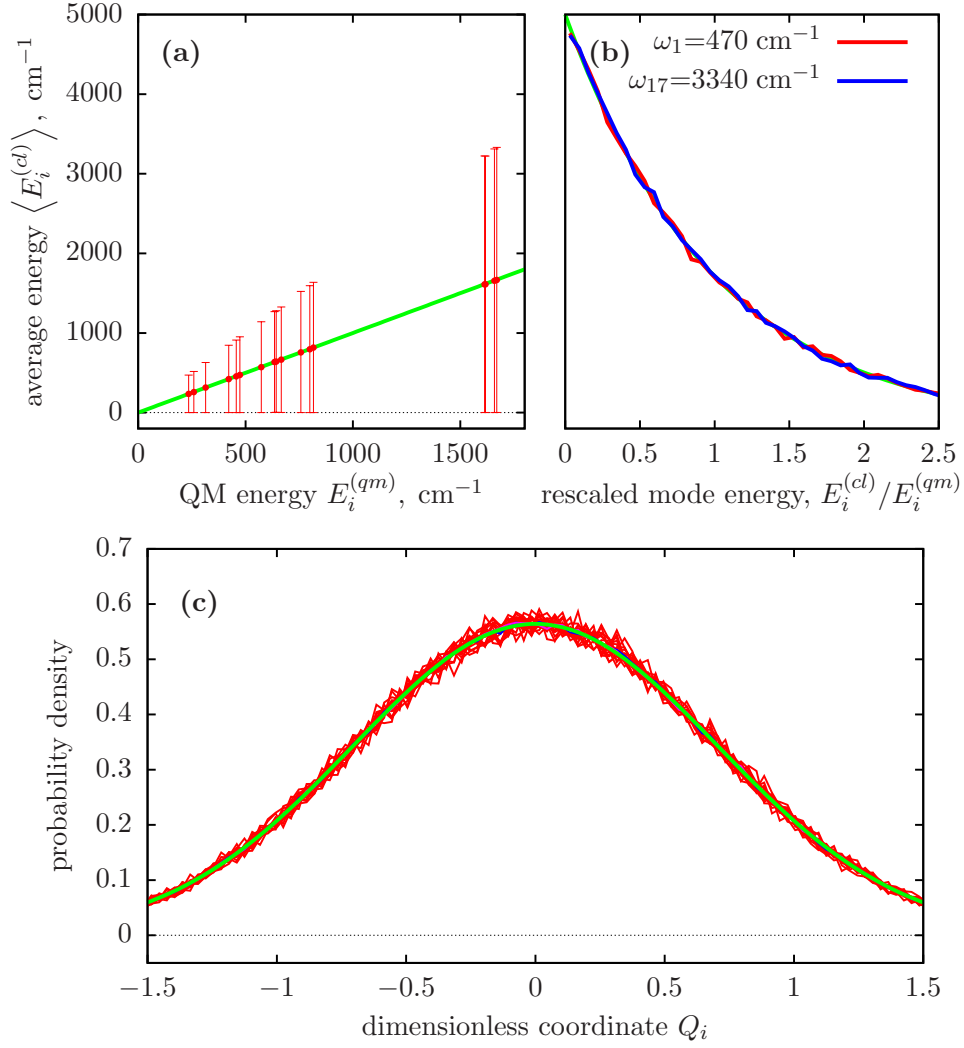


Figure S1: Wigner distribution for $\text{C}_2\text{H}_5\text{F}^\dagger$, 10^5 samples. Panel (a): average mode energies and standard deviations. Panel (b): rescaled energy distributions for the lowest and highest frequency modes. Panel (c): Q_i distributions for all modes. The green lines mark the exact QM energies and distributions, respectively.

S2 One mode harmonic oscillator

Table S1: Results obtained with different methods and parameters for the single mode oscillator. $N_S = 10^7$.

method	$E_i^{(cl)}$ AURE	$E_i^{(cl)}$ ARSTD	$\langle Q^2 \rangle =$ $\langle P^2 \rangle$	$\langle Q^4 \rangle =$ $\langle P^4 \rangle$
Wigner	0.000	1.00	0.500	0.750
MOV, MTV, MMS	0.000	0.00	0.500	0.375
MS, $\sigma=0.2$	0.000	0.20	0.500	0.390
MS, $\sigma=0.3$	0.001	0.30	0.500	0.409
MS, $\sigma=0.4$	0.007	0.39	0.503	0.438
MS, $\sigma=0.5$	0.003	0.47	0.502	0.460
MS, $\sigma=0.6$	0.012	0.53	0.506	0.491
MS, $\sigma=0.8$	0.020	0.63	0.510	0.540

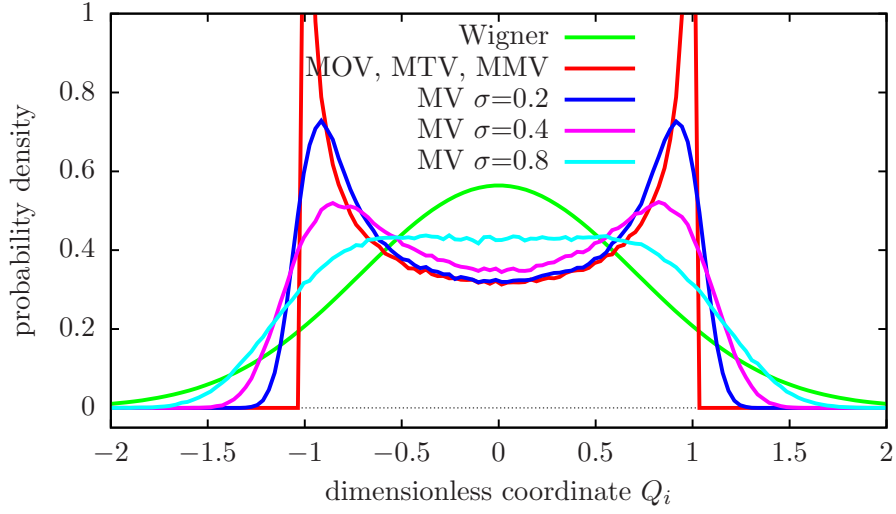


Figure S2: Q_i distributions for the single mode harmonic oscillator, obtained with the different sampling methods.

S3 Combined MMS sampling

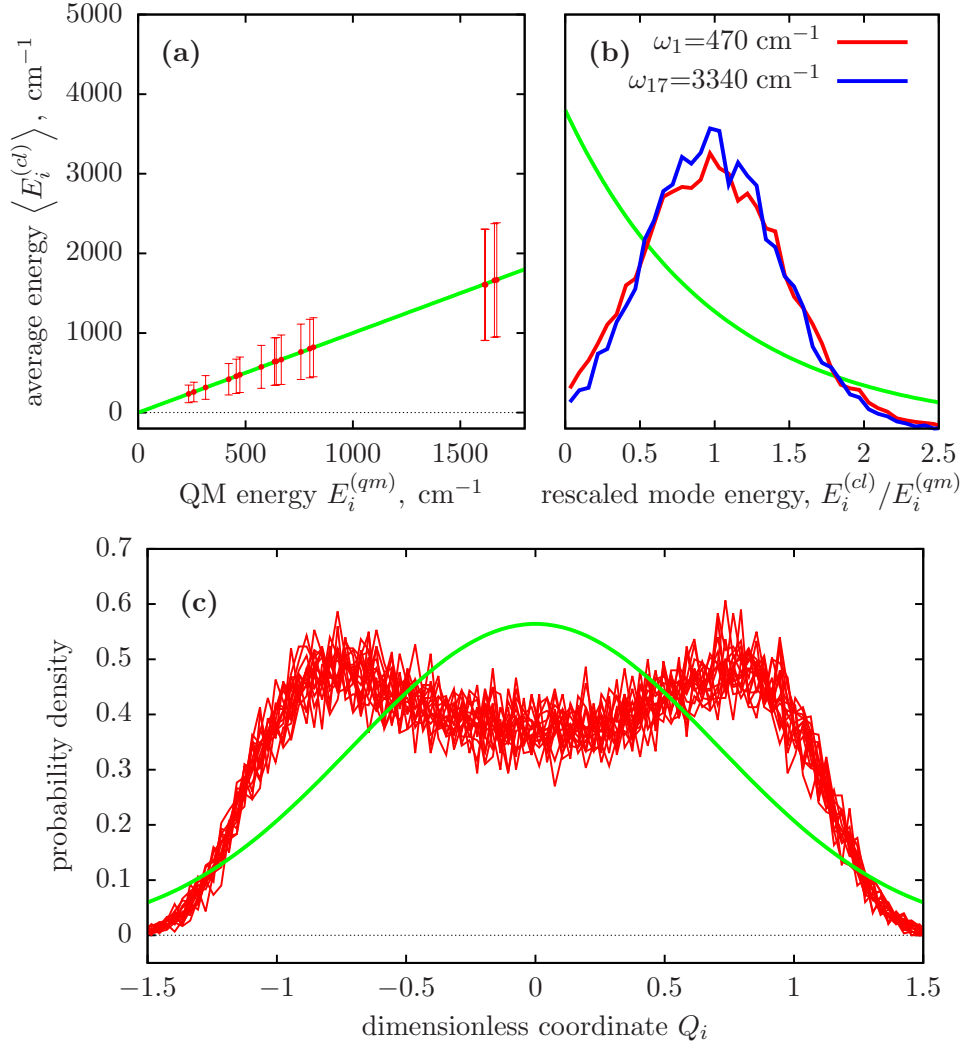


Figure S3: Sampling algorithm MMS for $\text{C}_2\text{H}_5\text{F}^\ddagger$. Bias parameter $\sigma = 0.5$, $N_S = 10^4$. Panel (a): average mode energies and standard deviations. Panel (b): rescaled energy distributions for the lowest and highest frequency modes. Panel (c): Q_i distributions for all modes. The green lines mark the exact QM energies and distributions, respectively.