University of Stuttgart
Institute for Theoretical Physics I

Johns Hopkins University

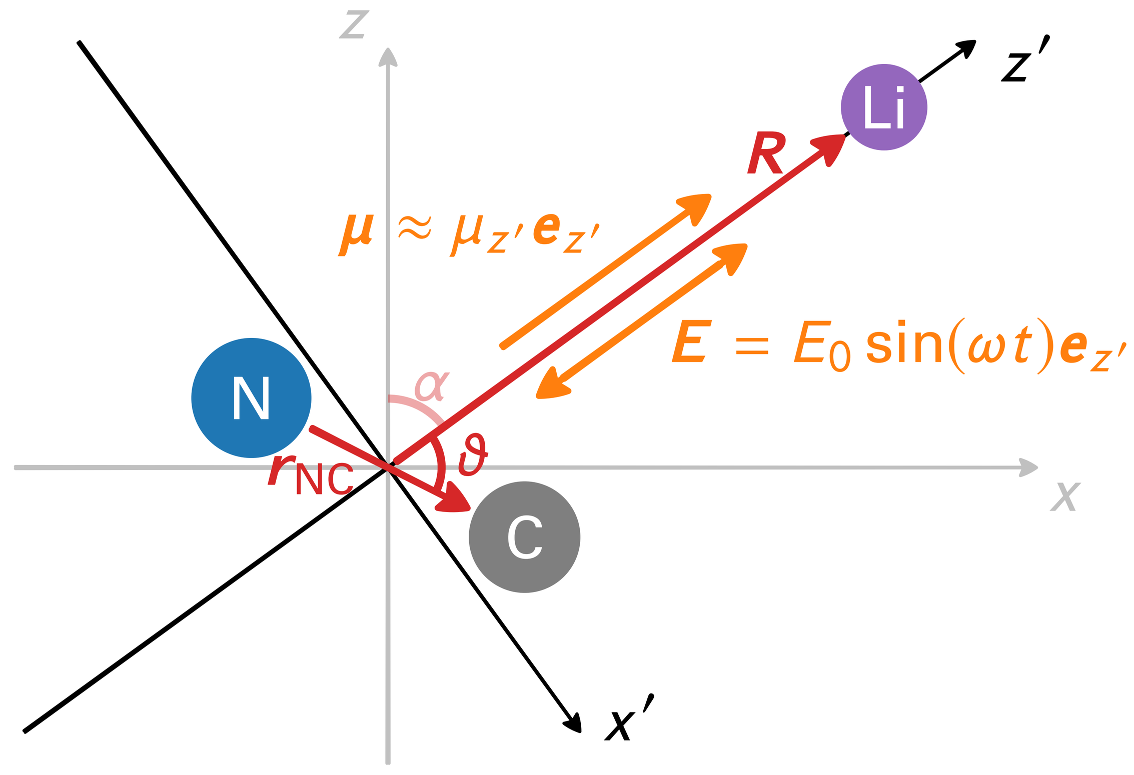
Transition State Theory in Driven Systems

Johannes Reiff, Jörg Main, and Rigoberto Hernandez

Applications

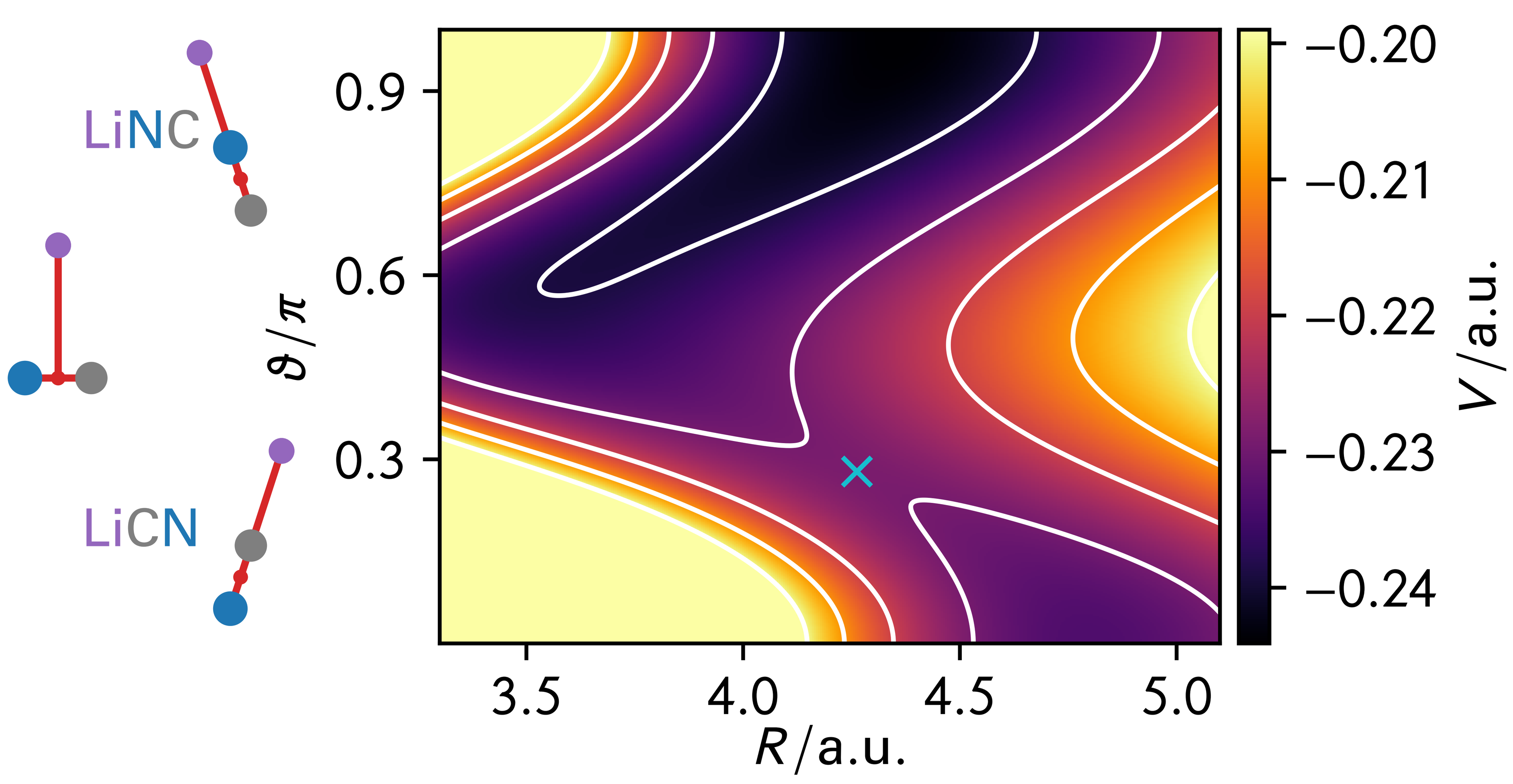
Abstract: Transition state theory has wide applicability, from chemical reactions to celestial mechanics. We use it to determine the stability of two such systems.

LiNC ⇌ LiCN Isomerization Reaction



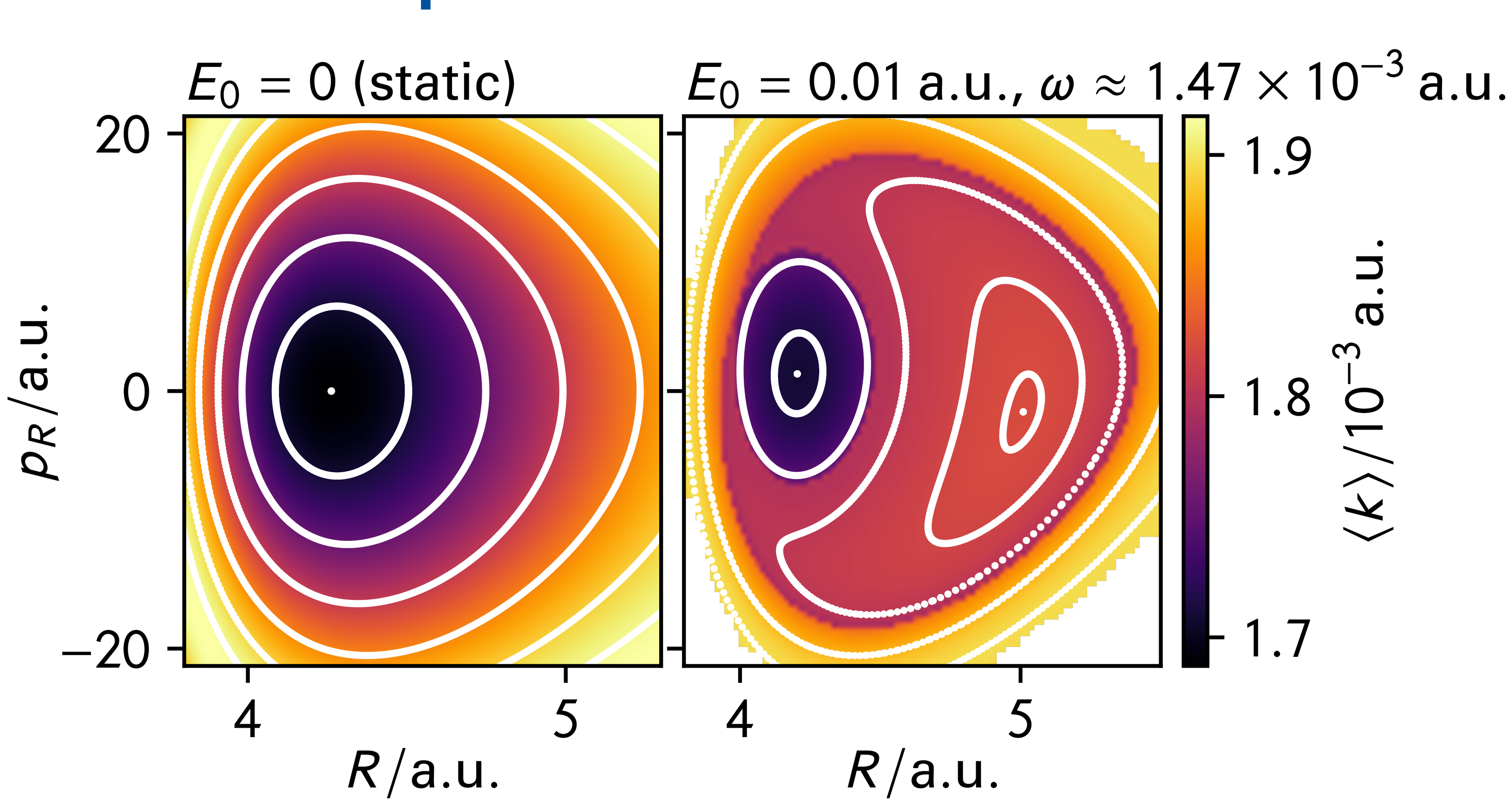
$$\mathcal{H} = \left[\frac{1}{\mu_1 R^2} + \frac{1}{\mu_2 r_{NC}^2} \right] \frac{p_\vartheta^2}{2} + \frac{p_R^2}{2\mu_1} + V(\vartheta, R) - \boldsymbol{\mu}(\vartheta, R) \cdot \boldsymbol{E}(t)$$

LiCN: Potential Surface



The dipole moment $\mu_{z'}$ is used to drive the effective potential.

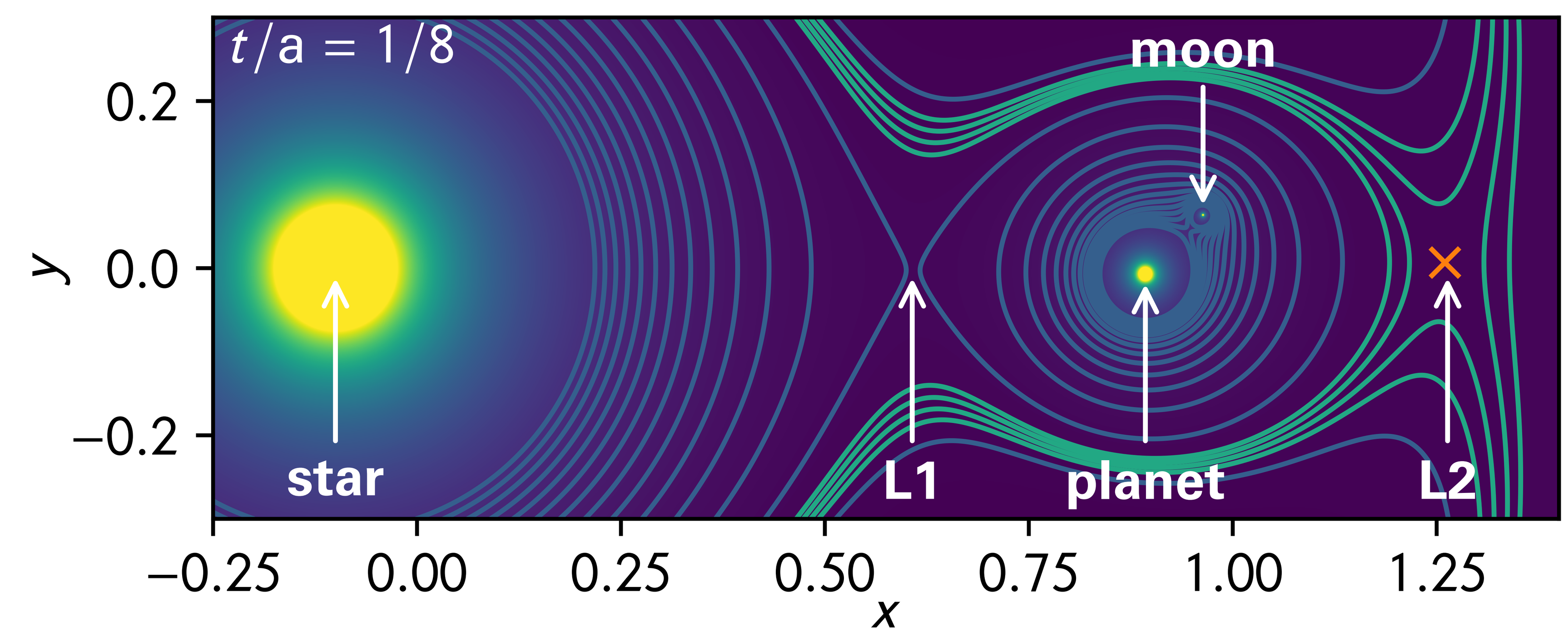
LiCN: Phase Space Structure



Driving creates new fixed points (FPs) via a bifurcation. The average decay rate at elliptic FPs is extremal.

M. Feldmaier, J. Reiff, R. M. Benito, F. Borondo, et al., J. Chem. Phys. **153**, 084115 (2020)

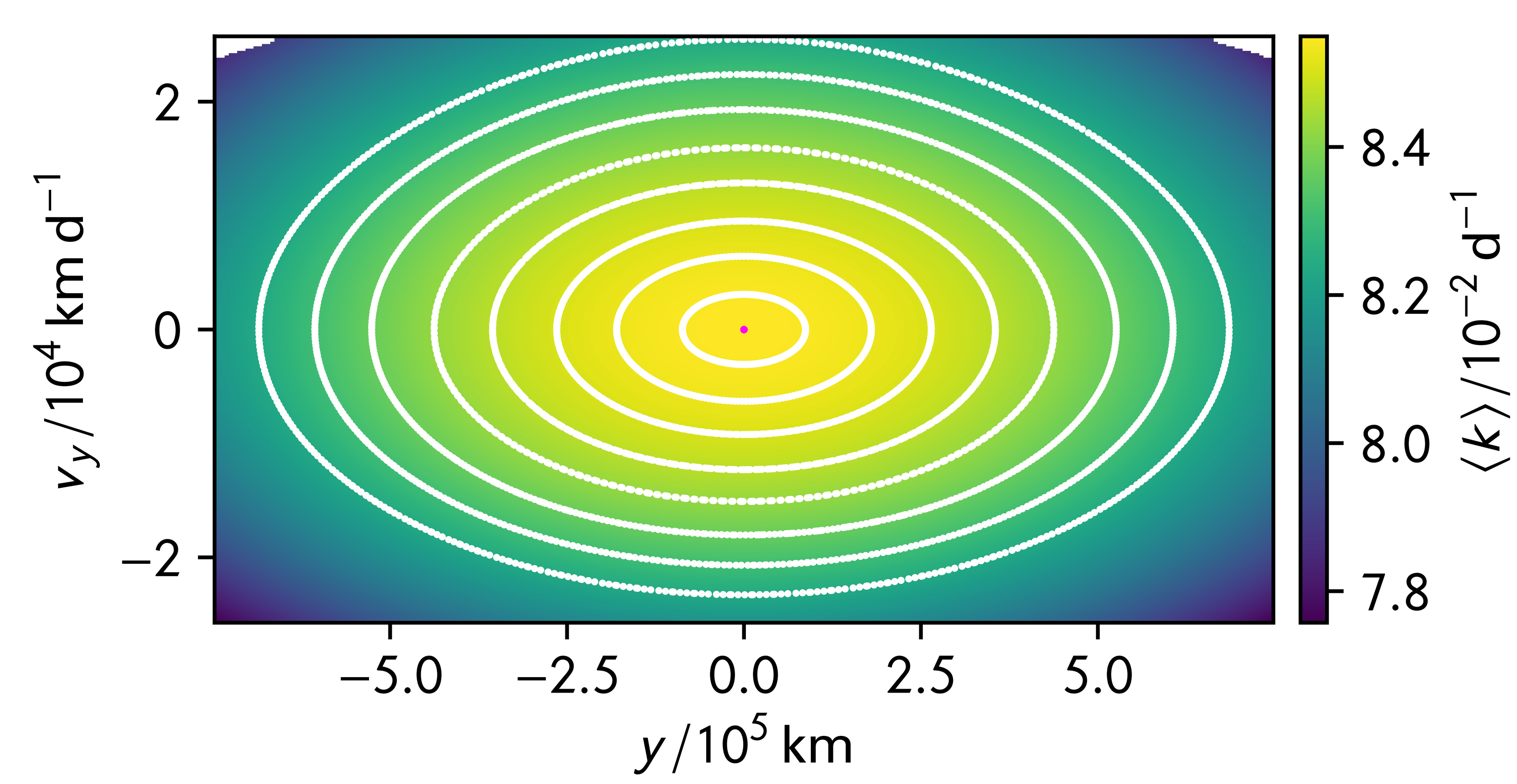
Bicircular Restricted Four-Body Problem (BCR4BP)



$$-V_{\mathrm{eff}}(\boldsymbol{r}) = \Omega(\boldsymbol{r}) = \frac{r^2}{2} + \frac{1-\mu}{|\boldsymbol{r} - \boldsymbol{R}_{\mathrm{S}}|} + \frac{\mu(1-\tilde{\mu})}{|\boldsymbol{r} - \boldsymbol{R}_{\mathrm{P}}|} + \frac{\mu\tilde{\mu}}{|\boldsymbol{r} - \boldsymbol{R}_{\mathrm{M}}|}$$

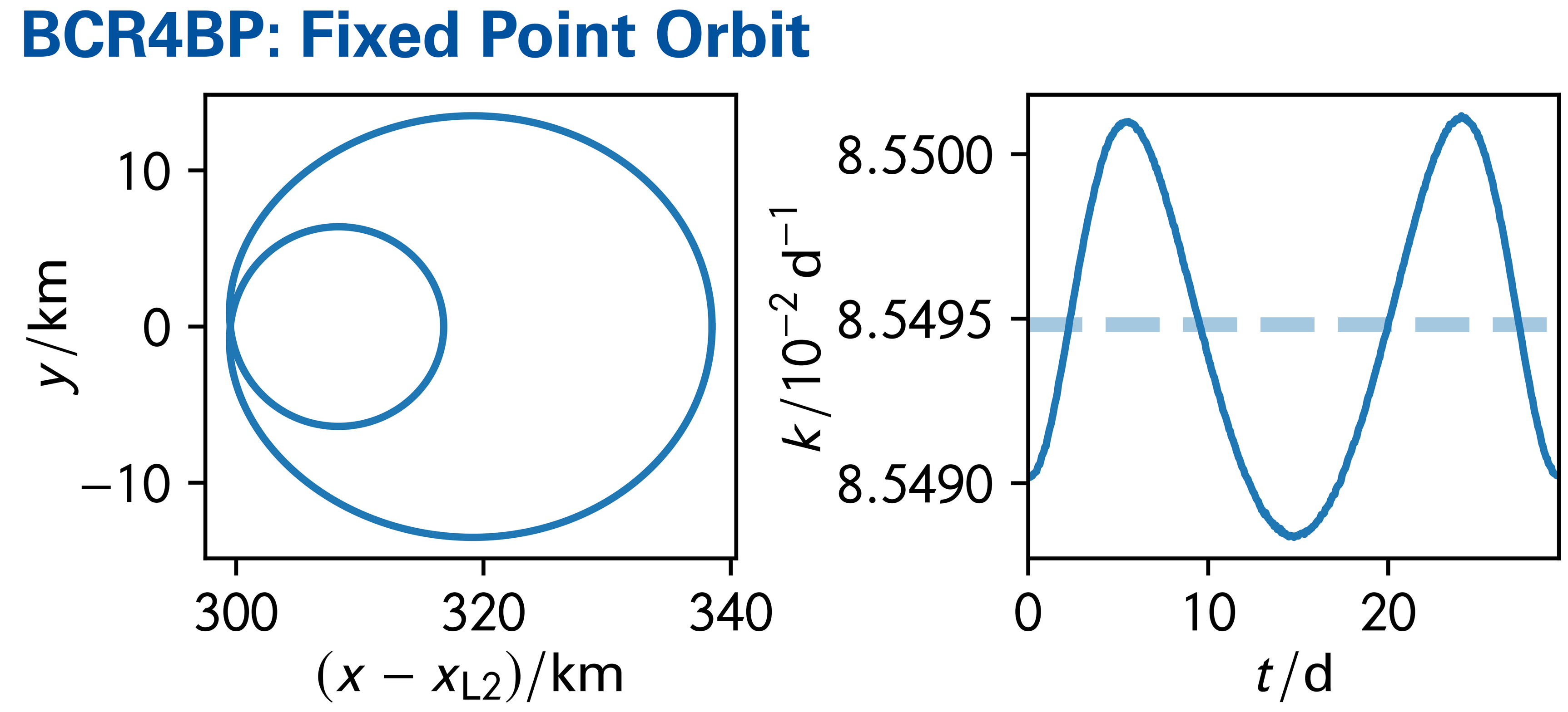
$$\ddot{x} - 2\dot{y} = \frac{\partial \Omega}{\partial x} \qquad \ddot{y} + 2\dot{x} = \frac{\partial \Omega}{\partial y}$$

BCR4BP: Phase Space Structure Around L2



Large orbits around L2 are more stable and, therefore, use less fuel than small orbits.

BCR4BP: Fixed Point Orbit



The L2 corresponds to an extended orbit when a moon is included in the model.

J. Reiff, J. Zatsch, J. Main, and R. Hernandez, Commun. Nonlinear Sci. Numer. Simul. **104**, 106053 (2022)

Founded by the DFG, the NSF, and the EU's Horizon 2020 Program (TraX).