Supplemental Material for

"Role of molecular bend angle and biaxiality in the stabilization of the twist-bend nematic phase"

Wojciech Tomczyk and Lech Longa

Institute of Theoretical Physics, Jagiellonian University, Łojasiewicza 11, 30-348 Kraków, Poland

Free energy f (eqn (12) in main manuscript) is minimized with respect to four parameters: q_0, q_2, θ and k, whereas adjustable are χ and λ. Here, we present selected exemplary results concerning the confirmation that the acquired states are equilibrium states. As initial parameters we take those that were obtained through direct minimization of eqn (12) (in main manuscript) for $t^* = 0.22$. Onward, we plot the evolution of free energy in (q_0, q_2) and (k, θ) domain for representative temperatures t^*.

Fig.S.1 ($\chi = 130^\circ$) and Fig.S.2 ($\chi = 140^\circ$) illustrate results for $\lambda = 0$. Columns (A) and (B) present contour plots of free energy in (q_0, q_2) and (k, θ) domain for twist-bend nematic (N_{TB}) state, while column (C) presents contour plots of free energy in (q_0, q_2) domain for nematic (N) state $\big(k = \theta = 0\big)$. The parameters from direct minimization for $t^* = 0.22$ are:

$\chi = 130^\circ$ $(\lambda = 0)$

- $q_0 = 0.68$, $q_2 = 0$, $k = 1$ and $\theta = 34^\circ$,

$\chi = 140^\circ$ $(\lambda = 0)$

- $q_0 = 0.68$, $q_2 = 0$, $k = 0.56$ and $\theta = 29^\circ$,

and they remain as fixed. Therefore, we have:

for Fig.S.1

- in column (A): fixed $\chi = 130^\circ$, $\lambda = 0$, $k = 1$, $\theta = 34^\circ$ and t^*, plots are in (q_0, q_2) domain;
- in column (B): fixed $\chi = 130^\circ$, $\lambda = 0$, $q_0 = 0.68$, $q_2 = 0$ and t^*, plots are in (k, θ) domain;
- in column (C): fixed $\chi = 130^\circ$, $\lambda = 0$, $k = 0$, $\theta = 0$ and t^*, plots are in (q_0, q_2) domain;

for Fig.S.2

- in column (A): fixed $\chi = 140^\circ$, $\lambda = 0$, $k = 0.56$, $\theta = 29^\circ$ and t^*, plots are in (q_0, q_2) domain;
- in column (B): fixed $\chi = 140^\circ$, $\lambda = 0$, $q_0 = 0.68$, $q_2 = 0$ and t^*, plots are in (k, θ) domain;
- in column (C): fixed $\chi = 140^\circ$, $\lambda = 0$, $k = 0$, $\theta = 0$ and t^*, plots are in (q_0, q_2) domain;

Fig.S.3 ($\chi = 130^\circ$) and Fig.S.4 ($\chi = 145^\circ$) depict results for $\lambda = 0.3$. Idea behind columns (A), (B) and (C) is the same as in Fig.S.1 and Fig.S.2. The parameters from direct minimization for $t^* = 0.22$ are:
$\chi = 130^\circ$ ($\lambda = 0.3$)

- $q_0 = 0.8$, $q_2 = 0.3$, $k = 1.81$ and $\theta = 25^\circ$,

$\chi = 145^\circ$ ($\lambda = 0.3$)

- $q_0 = 0.8$, $q_2 = 0.24$, $k = 1.7$ and $\theta = 17^\circ$,

and they remain as fixed. Therefore, we have:

for Fig.S.3

- in column (A): fixed $\chi = 130^\circ$, $\lambda = 0.3$, $k = 1.81$, $\theta = 25^\circ$ and t^*, plots are in (q_0, q_2) domain;
- in column (B): fixed $\chi = 130^\circ$, $\lambda = 0.3$, $q_0 = 0.8$, $q_2 = 0.3$ and t^*, plots are in (k, θ) domain;
- in column (C): fixed $\chi = 130^\circ$, $\lambda = 0.3$, $k = 0$, $\theta = 0$ and t^*, plots are in (q_0, q_2) domain;

for Fig.S.4

- in column (A): fixed $\chi = 145^\circ$, $\lambda = 0.3$, $k = 1.7$, $\theta = 17^\circ$ and t^*, plots are in (q_0, q_2) domain;
- in column (B): fixed $\chi = 145^\circ$, $\lambda = 0.3$, $q_0 = 0.8$, $q_2 = 0.24$ and t^*, plots are in (k, θ) domain;
- in column (C): fixed $\chi = 145^\circ$, $\lambda = 0.3$, $k = 0$, $\theta = 0$ and t^*, plots are in (q_0, q_2) domain;

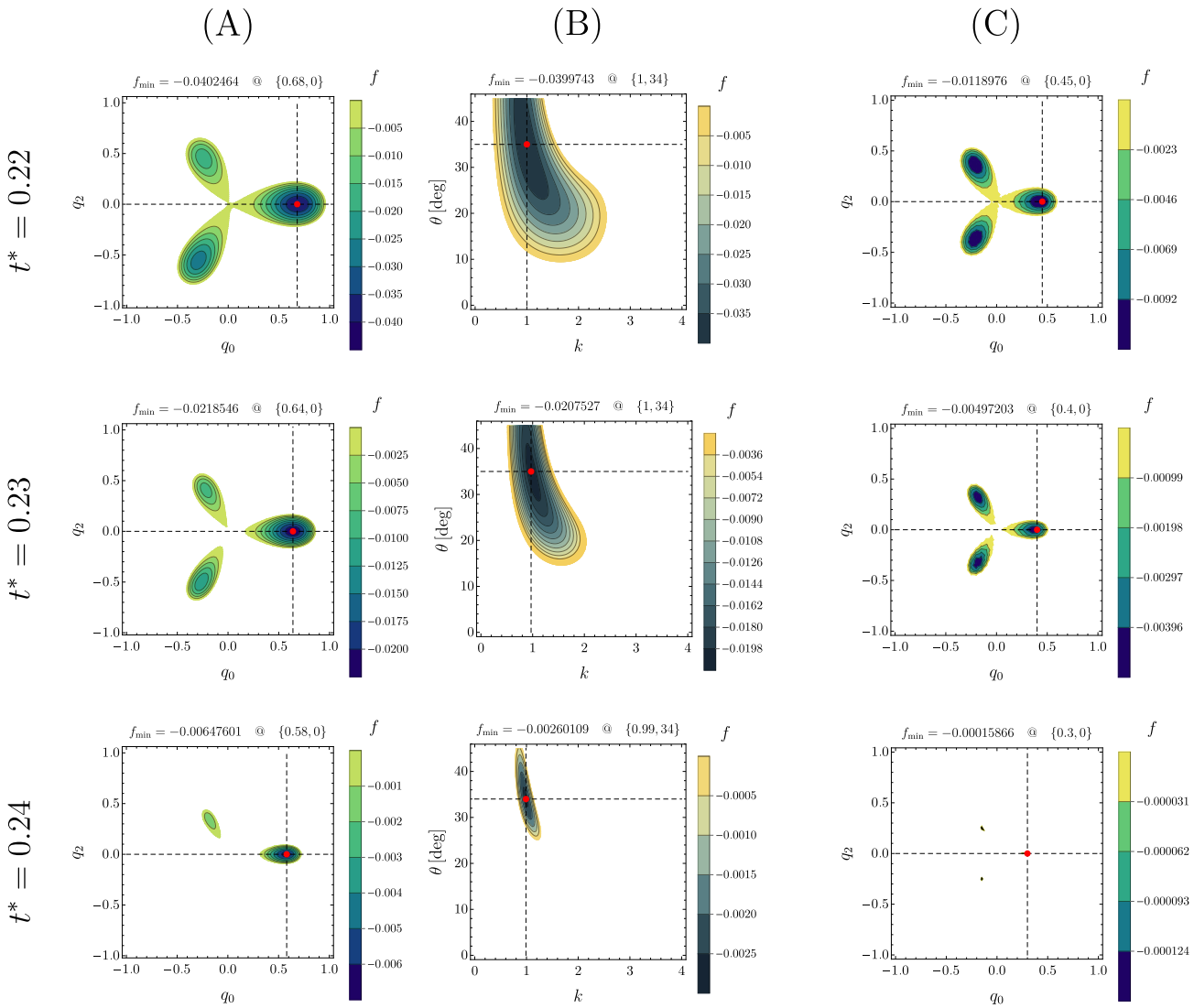

Figure S.1: Contour plots of free energy in (q_0, q_2) and (k, θ) domain for $\chi = 130^\circ$ and $\lambda = 0$ (*see the text of this Supplemental Material*). Above each contour plot is printed a set of numbers, which designate for what pair (q_0, q_2) or (k, θ) the lowest value of free energy is attained (red dot). White space in plots is associated with the area where $f \geqslant 0$. The resolution in (q_0, q_2) plots is 0.05 and in (k, θ) plots is 0.05 (for k) and 1° (for θ). According to the values of f in this scenario N_{TB} prevail over N_{U}.

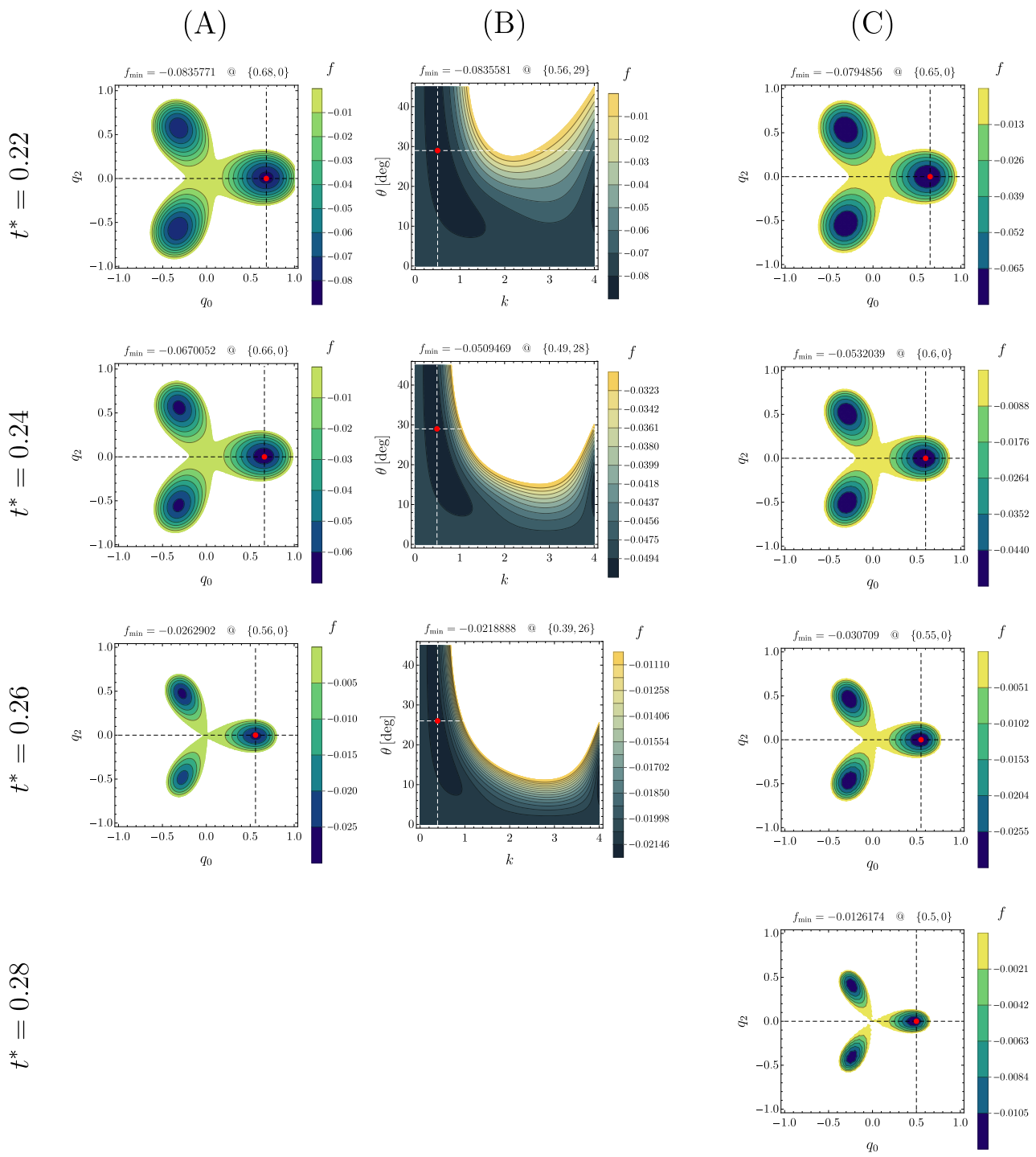

Figure S.2: Contour plots of free energy in (q_0, q_2) and (k, θ) domain for $\chi = 140^\circ$ and $\lambda = 0$ (*see the text of this Supplemental Material*). Above each contour plot is printed a set of numbers, which designate for what pair (q_0, q_2) or (k, θ) the lowest value of free energy is attained (red dot). White space in plots is associated with the area where $f \geqslant 0$. Lack of plots in column (A) and (B) for $t^* = 0.28$ indicate that for whole set of either (q_0, q_2) or (k, θ) $f \geqslant 0$ (N_{U} dominates). The resolution in (q_0, q_2) plots is 0.05 and in (k, θ) plots is 0.05 (for k) and 1° (for θ). According to the values of f in this scenario a phase transition between N_{TB} and N_{U} occurs.

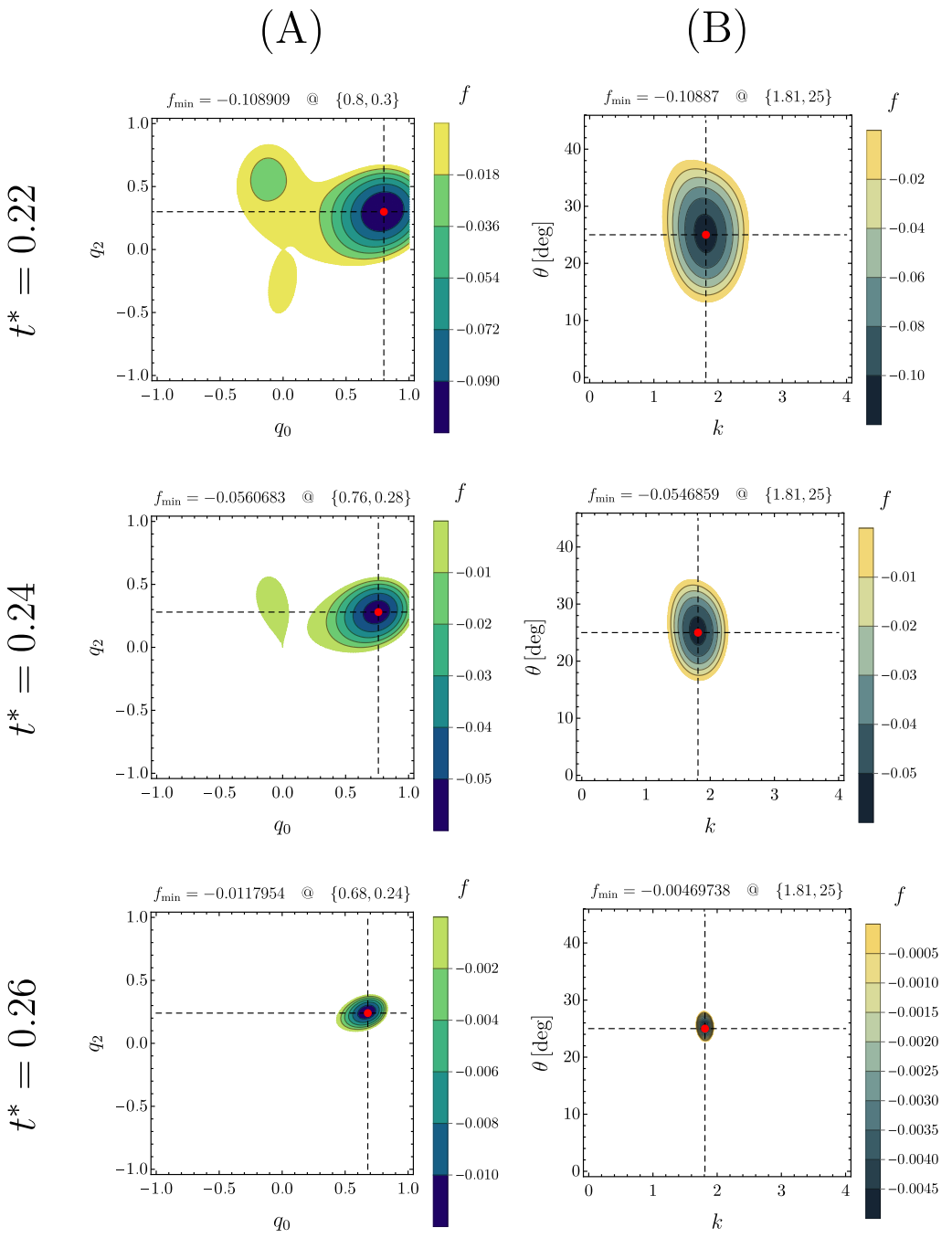

Figure S.3: Contour plots of free energy in (q_0, q_2) and (k, θ) domain for $\chi = 130^\circ$ and $\lambda = 0.3$ (*see the text of this Supplemental Material*). Above each contour plot is printed a set of numbers, which designate for what pair (q_0, q_2) or (k, θ) the lowest value of free energy is attained (red dot). White space in plots is associated with the area where $f \geqslant 0$. Lack of column (C) indicate that for whole set of (q_0, q_2) $f \geqslant 0$ ($N_{\mathrm{TB,B}}$ phase dominates). The resolution in (q_0, q_2) plots is 0.05 and in (k, θ) plots is 0.05 (for k) and 1° (for θ). According to the values of f in this scenario $N_{\mathrm{TB,B}}$ prevail over N_{U}.

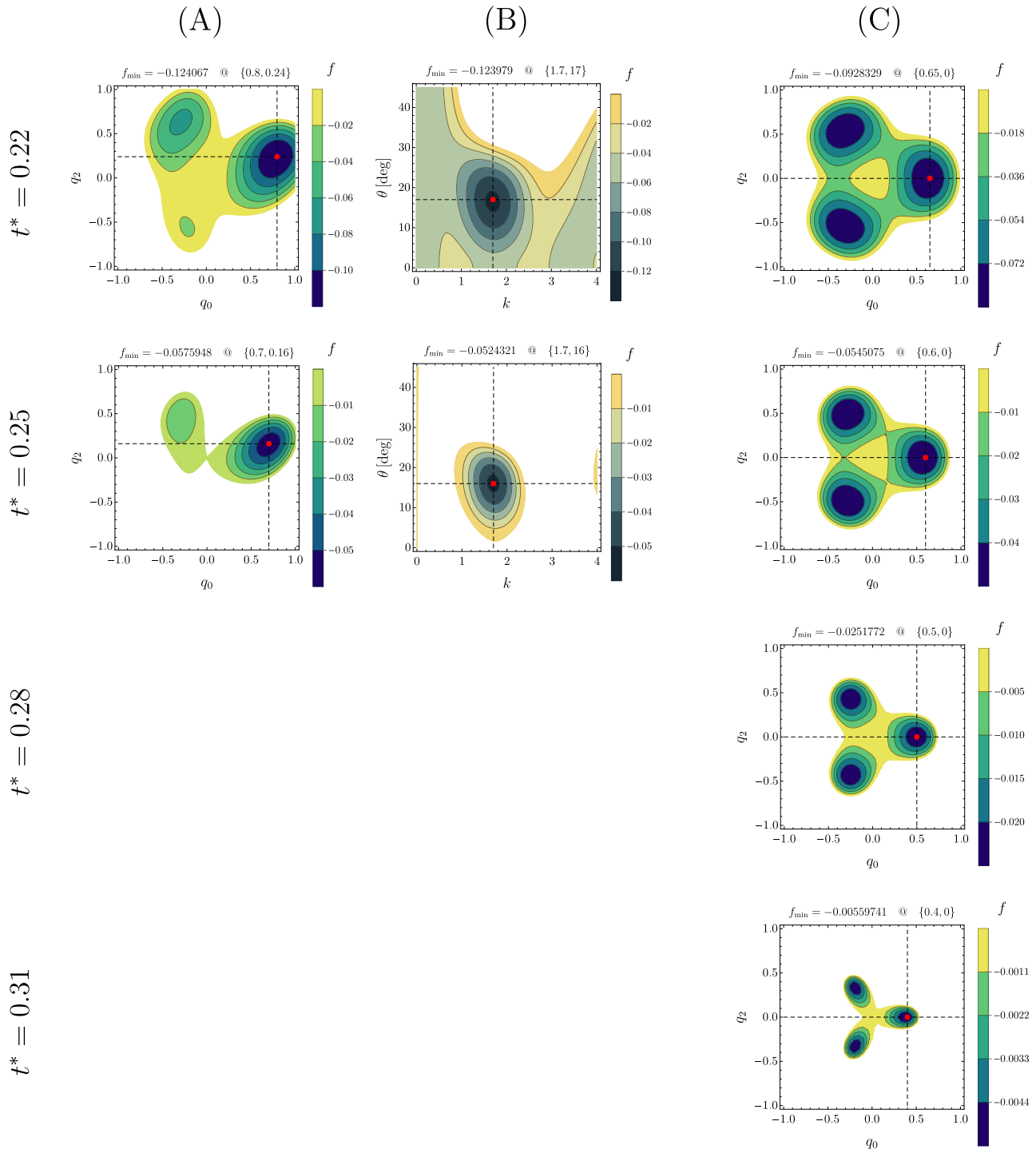

Figure S.4: Contour plots of free energy in (q_0, q_2) and (k, θ) domain for $\chi = 145^\circ$ and $\lambda = 0.3$ (*see the text of this Supplemental Material*). Above each contour plot is printed a set of numbers, which designate for what pair (q_0, q_2) or (k, θ) the lowest value of free energy is attained (red dot). White space in plots is associated with the area where $f \geqslant 0$. Lack of plots in column (A) and (B) for $t^* = 0.28$ and $t^* = 0.31$ indicate that for whole set of either (q_0, q_2) or (k, θ) $f \geqslant 0$ (N_{U} phase dominates). The resolution in (q_0, q_2) plots is 0.05 and in (k, θ) plots is 0.05 (for k) and 1° (for θ). According to the values of f in this scenario a phase transition between $N_{\mathrm{TB,B}}$ and N_{U} occurs.