1 Geometrical method

Let us have a Hamiltonian system with the standard kinetic term and a potential depending only on coordinates $\boldsymbol{x} = (x^i)$

$$H = \frac{1}{2M}\boldsymbol{p}^2 + V(\boldsymbol{x}). \tag{1}$$

Then the conjecture of the paper [1] is: *When at least one of the eigenvalues λ_i of the matrix*

$$\mathcal{V}_{ij}(\boldsymbol{x}) = \frac{3}{M^2\boldsymbol{v}^2}\frac{\partial V}{\partial x^i}\frac{\partial V}{\partial x^j} + \frac{1}{M}\frac{\partial V}{\partial x^i \partial x^j} \tag{2}$$

is negative inside the energetically allowed part of the configuration space, then the system is unstable and chaotic trajectories can be present. In practice this means that one has to compute (i) the region where the smallest eigenvalue $\lambda_{\min}$ of the matrix $\mathcal{V}$ is negative, and (ii) the region of the kinematically accessible area. If these two regions have an intersection, chaotic trajectories can appear. Specifically, for a 2D system one solves (in general numerically) two equations

$$\lambda_{\min} \equiv \frac{1}{2}\left[\mathcal{V}_{xx} + \mathcal{V}_{yy} + \sqrt{(\mathcal{V}_{xx} + \mathcal{V}_{yy})^2 - 4\mathcal{V}_{xy}^2}\right] = 0 \tag{3}$$

$$V = 0 \tag{4}$$

in the plane (x, y) and then searches for the intersection of the curves corresponding with each of the equations.

But one can be more clever. In the Geometric Collective Model, the following equivalence can been proven: *If the negative region of the smallest eigenvalue $\lambda_{\min}$ crosses the border of the kinematically accessible area at a given energy, then this affected part of the border is concave, i.e. dispersing.* This concave criterion is easy to use because it only requires to calculate the curve $V(x, y) = 0$, and then its second derivative in order to determine whether or not it is concave in some of its part. Since it can also occur that the region of a negative eigenvalue $\lambda_{\min}$ is fully inside the kinematically allowed area, resulting in instability in spite of the fact that the border is convex along all its length, the concave criterion must be employed for all equipotential contours *below* the given energy in order to assess the stability correctly. This is not a big complication because one is usually interested in the stable–unstable crossover at low energies, so the stability is calculated from the minimum energy where the system is usually perfectly stable (and thus not affected by negative λ_i intruders in the accesible region) and when once the curve $V = 0$ becomes concave, the crossover energy E_c is found.

In the Creagh-Whelan model

$$H = \frac{1}{2}(p_x^2 + p_y^2) + (x^2 - 1)^2 + Ax + Bxy^2 + Cx^2y^2 + Dy^2, \tag{5}$$

the connection between the curvature of the kinematically accessible border and the region of negative $\lambda_{\min}$ is also valid, see an example in Figure 1. The simple form of the Creagh-Whelan potential allows one to calculate the border $V = 0$ analytically:

$$y(x) = \pm\sqrt{\frac{E - (x^2 - 1)^2 - Ax}{Bx + Cx^2 + D}} \tag{6}$$

Taking only the upper part of the border (+ sign), convex interior corresponds to the concave form of the function $y(x)$ with, $y''(x) < 0$ and vice versa.

An example of the convex-shape and concave-shape distribution as a function of the control parameter A in an assymetric ($B \neq 0$) configuration of the Creagh-Whelan model is shown in

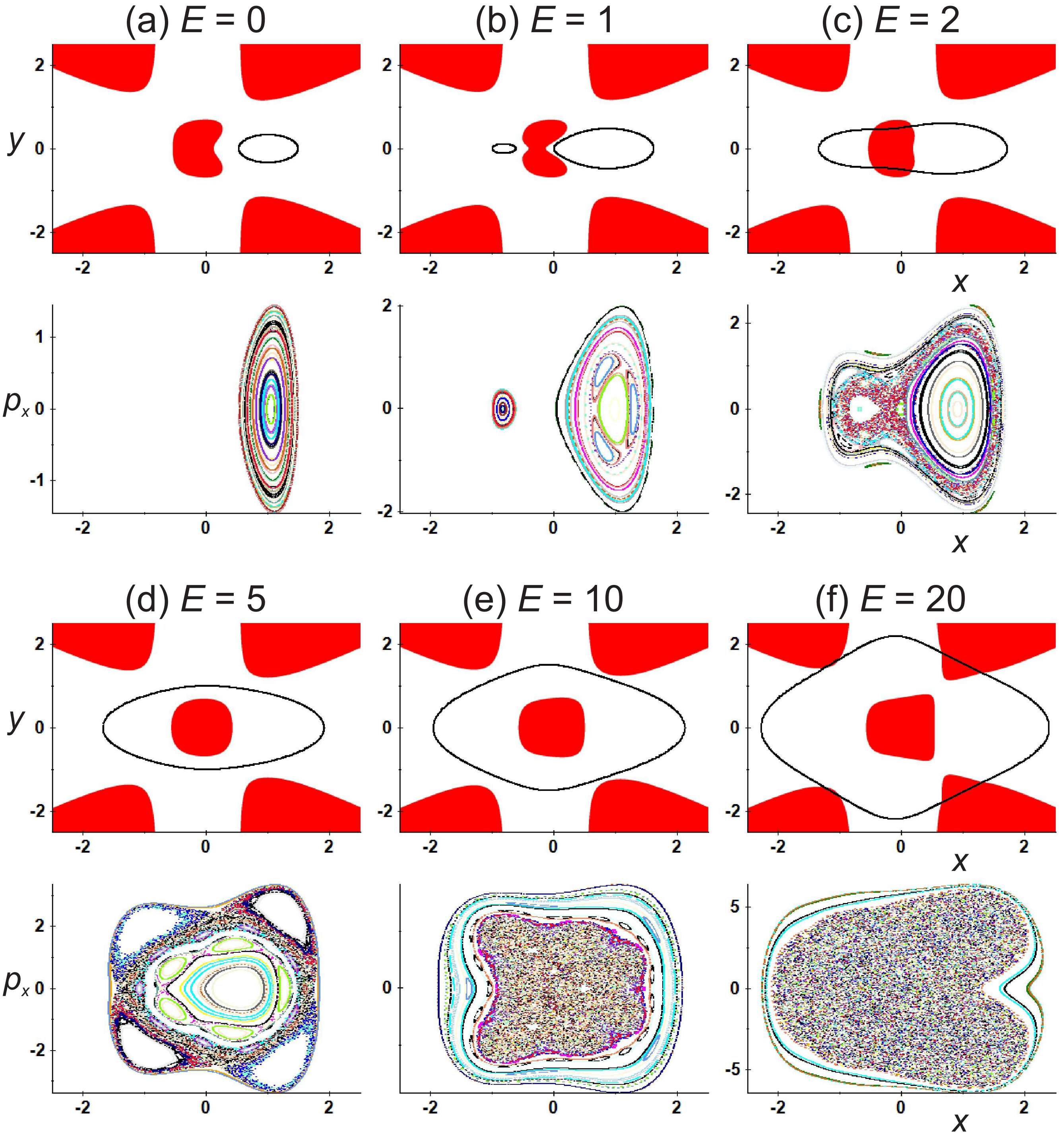

Figure 1: Kinematically accesible region (black curve), regions of negative values of the eigenvalue $\lambda_{\min}$ (red areas), and corresponding Poincaré sections for the Creagh-Whelan model with $A = -1, B = 1, C = D = 4$. Energies are indicated in the caption of each doublepanel. Note that there are several convex-concave and concave-convex transitions, but chaotic trajectories appear above the first one at energy $E \approx 1.2$ and remain for all higher energies, even though surrounded by a completely convex border, as in panels (d)–(e).

Figure 2(a). By going up in energy the accessible border can change its shape from fully convex to partly concave and back several times. However, only the first convex-concave crossover is significant for the stability-instability transition. If a fully convex encircling line appears again higher in energy, it always has some concave equipotential contours underneath that prevents stability. That is in full agreement with the Geometry method that predicts instability due to surviving regions of negative $\lambda_{\max}$ encircled by the energy border, see Figure 1(d)–(e).

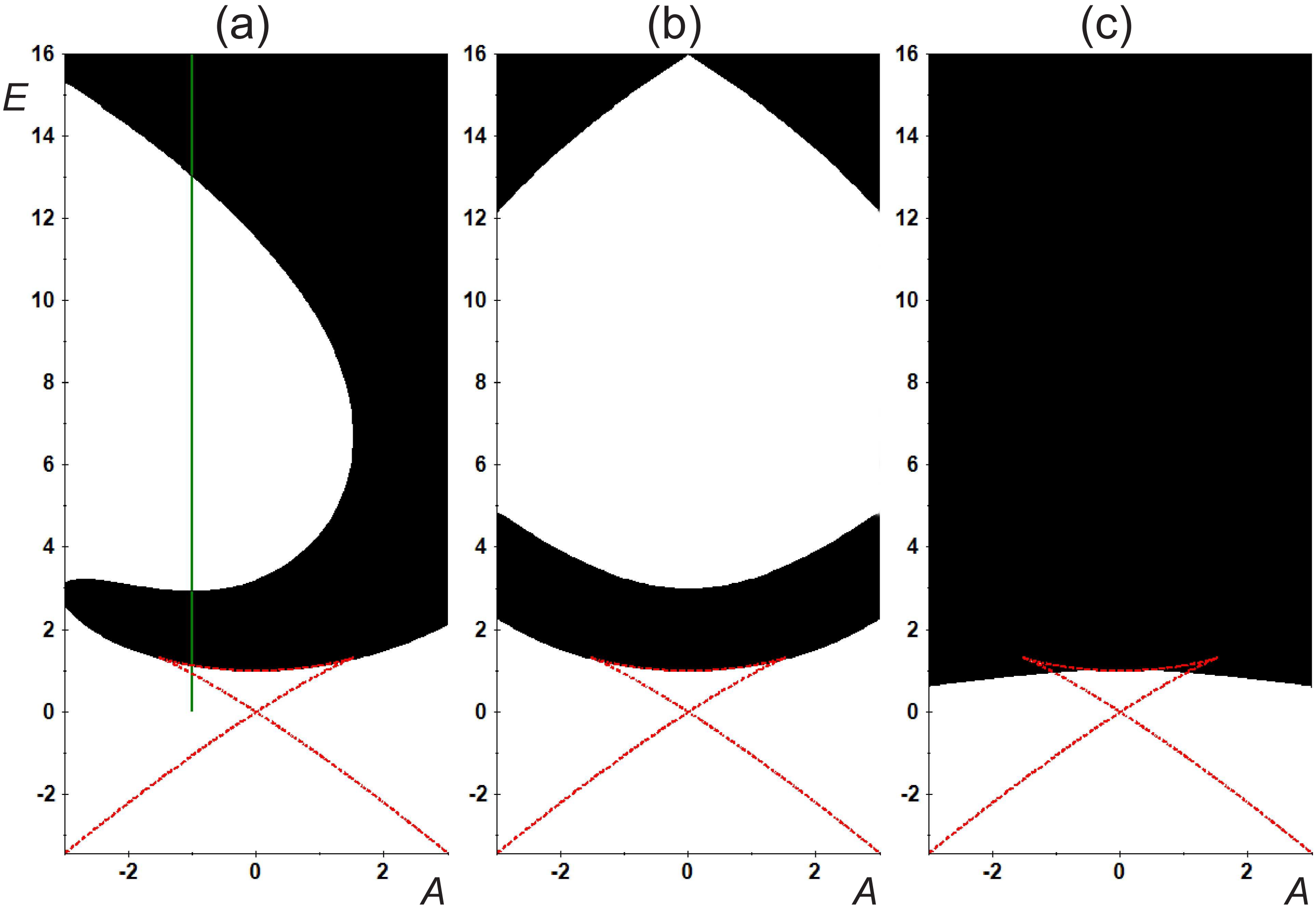

Figure 2: Regions of a completely convex (white) and partly concave (black) border line for the Creagh-Whelan model with (a) $B = 1, C = D = 4$ (asymmetric), (b) $B = 0, C = D =$ arbitrary (symmetric), (c) $B = 0, C = 39, D = 1$ (symmetric, strongly elongated along the y-axis). Red dashed lines show the position of the critical triangle and correspond with the energy of the two minima and the saddle point of the potential (positions of the minima and the saddle point do not depend on the parameters B, C, D provided the confinement conditions $C, D > 0$, $\sqrt{4CD} > B$ is fulfilled). (a) The green line indicate the value of parameter A used in Figure 1. Note that the first convex-concave transition, *i.e.* the stability-instability transition, nicely coincide with the position of the saddle point in panels (a)–(b).

Additional observations:

- If $B = 0$ (symmetic configuration) and $C = D$, then the convex-concave transition is independent of their value. An example is shown in Figure 2(b), and further on in Figure 3(a)–(e).

- If $C \leq D$, then the first concave equipotential contour appears very close to the energy of the saddle point, and hence the saddle point gives approximately the dividing barrier between the stable and unstable dynamics. On the other hand, for $C \gg D$ the potential becomes strongly stretched along the y-axis, resulting in deformed partly concave equipotential contours deep below the saddle point in each individual well, see Figure 2(c). Note that there is a need of some asymmetry, induced in this example by $A \neq 0$.

- If $B \neq 0$, the potential is even more asymmetric and a significant part of the critical triangle can be covered by an unstable region. This occurs when $B \lessapprox \sqrt{4CD}$. One of the most interesting configuration belonging to this group is that of one minimum stable and the other highly unstable. An example is shown in Figure 3(l).

Finally, the stable-unstable border determined by the Geometrical method is drawn together with the map of regularity f_{reg} and presented in Figure 3. Some mismatch between f_{reg} and the stable-unstable line is observed in panel (a) (the system is regular at both sides of the graph, well inside the unstable region) and in panels (i)–(j) (chaotic trajectories appear already below the unstability line).

The results are also presented on the web page http://www.pavelstransky.cz/cw.php (f_{reg} is there now in Figure 3, and also together with the level dynamics in Figure 6).

References

[1] L. Horwitz, Y.B. Zion, M. Lewkowicz, M. Schiffer, and J. Levitan, *Phys. Rev. Lett.* **98**, 234301 (2007).

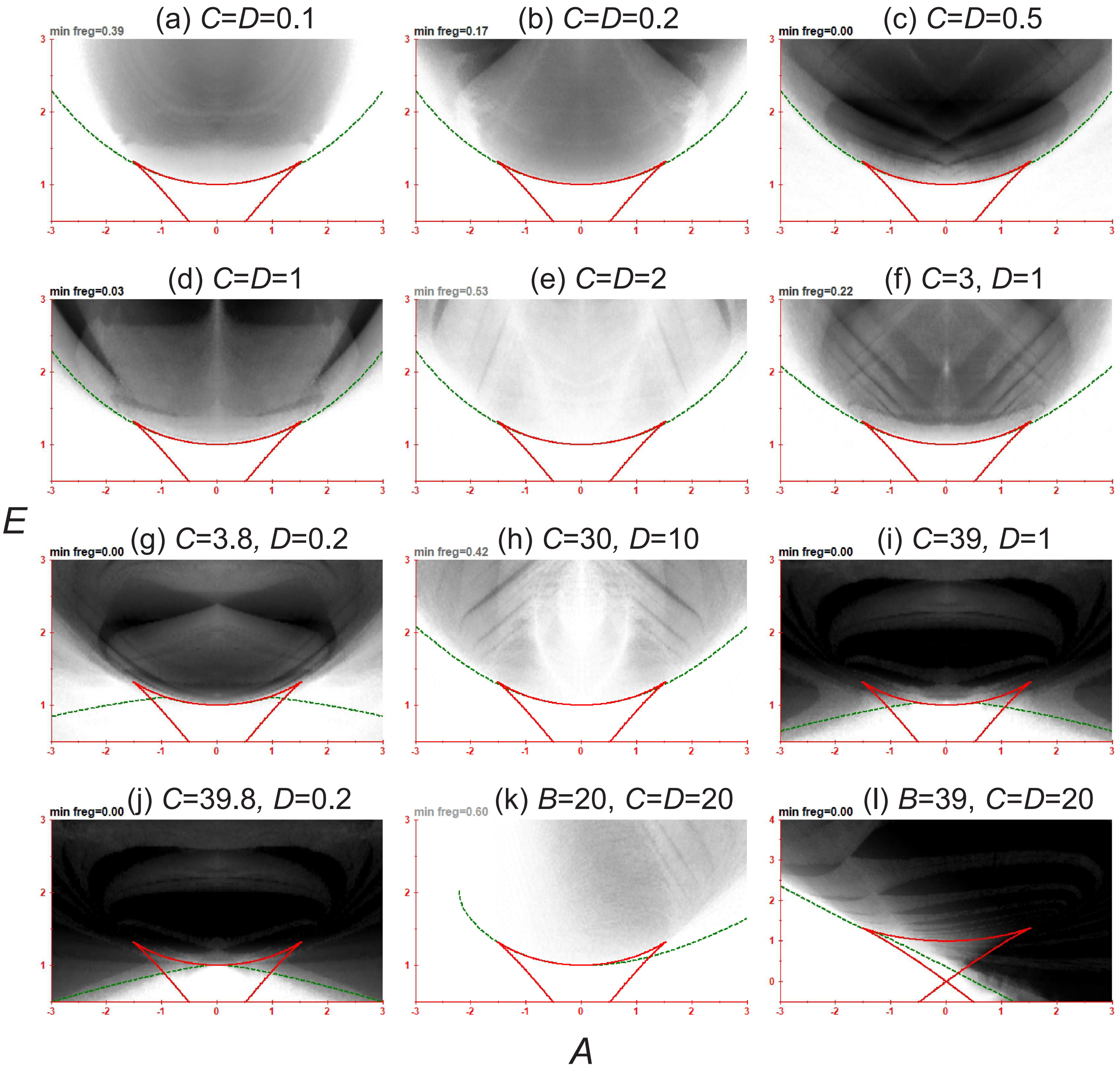

Figure 3: Fraction of regularity f_{reg} of the Creagh-Whelan model, calculated from the $y = 0$ Poincaré section for each of the (240×140) points in the (A, E) plane, and coded in shades of gray (black - fully caotic, white - fully regular). Panels (a)–(j) correspond with the symmetric $B = 0$ configuration, panels (k)–(l) show asymmetric $B = 20$ configuration. The values of the remaining parameters are given in the captions of each panel. Red solid line surrounds the critical triangle, green dashed line show the lowest-lying convex-concave (*i.e.* stability-instability) transition. Note that this border line does not change in panels (a)–(e), in agreement with the statement given in the main text.