1 GCM adapted for the study of variable rigidity

1.1 Hamiltonian

$$H = T + V = \frac{1}{2K}\left(\pi_\beta^2 + \frac{1}{\beta^2}\pi_\gamma^2\right) + A\beta^2 + B\beta^3 f(\gamma) + C\beta^4 \tag{1}$$

A, B, C, K are adjustable parameters (with the same meaning as in the GCM). The function $f(\gamma)$ is imposed to have the following properties:

1. $f(\gamma)$ is analytic and periodic with the period 2π: $f(\gamma) = f(\gamma + 2j\pi)$.
2. On the interval $[0, 2\pi)$, $f(\gamma)$ has only one minimum $f(\gamma_{\min}) = -1$ and one maximum $f(\gamma_{\max})$=1.
3. The range of values of $f(\gamma)$ is $[-1, 1]$.
4. The function is symmetric around the minimum:

$$f(\gamma_{\min} + \gamma) = f(\gamma_{\min} - \gamma).$$

The potential given by (1) has two minima at

$$\beta_1 = 0 \qquad \text{(spherical)} \tag{2}$$

$$\beta_2 = \frac{3B + \sqrt{9B^2 - 32AC}}{8C}, \gamma_{\min} \qquad \text{(deformed)} \tag{3}$$

and a barrier between them at

$$\beta_B = \frac{3B - \sqrt{9B^2 - 32AC}}{8C} \tag{4}$$

provided that $A, B, C > 0$, $9B^2 > 32AC$.

The spherical–deformed shape phase transition occurs for $B^2 = 4AC$. On the phase transition, both minima have the same depth $\bar{V}(\bar{\beta}_1 = 0) = \bar{V}(\bar{\beta}_2 = \sqrt{A/C}) = 0$[1] and they are separated by the barrier $\bar{V}(\bar{\beta}_B = \frac{1}{2}\sqrt{\frac{A}{C}}) = A^2/16C$. The Taylor expansion at the deformed minimum in the direction β is

$$\bar{V}(\beta) = A(\beta - \bar{\beta}_2)^2 + O(\beta - \bar{\beta}_2)^3. \tag{5}$$

By comparing the quadratic term with the Hamiltonian of the harmonic oscillator, the frequency of small β vibrations is

$$\bar{\Omega}_\beta = \sqrt{\frac{2A}{K}}, \tag{6}$$

where K is the mass parameter of the Hamiltonian. We will be interested in the ratio of β and γ frequencies (the "rigidity ratio") defined as

$$\bar{R} = \frac{\bar{\Omega}_\gamma}{\bar{\Omega}_\beta}, \tag{7}$$

where

[1]Quantities expressed on the phase transition $B^2 = 4AC$ are marked with the bar in the whole text.

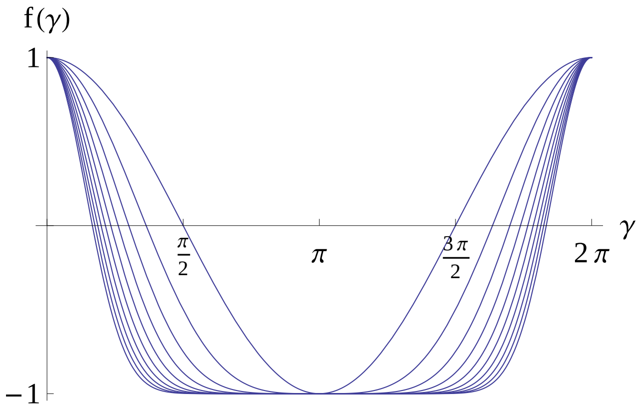
1. $R < 1$ for γ-soft cases,
2. $R > 1$ for γ-rigid cases.

Note, however, that in general this ratio changes when one moves out from the critical point. This will be discussed briefly in Sec. 1.4

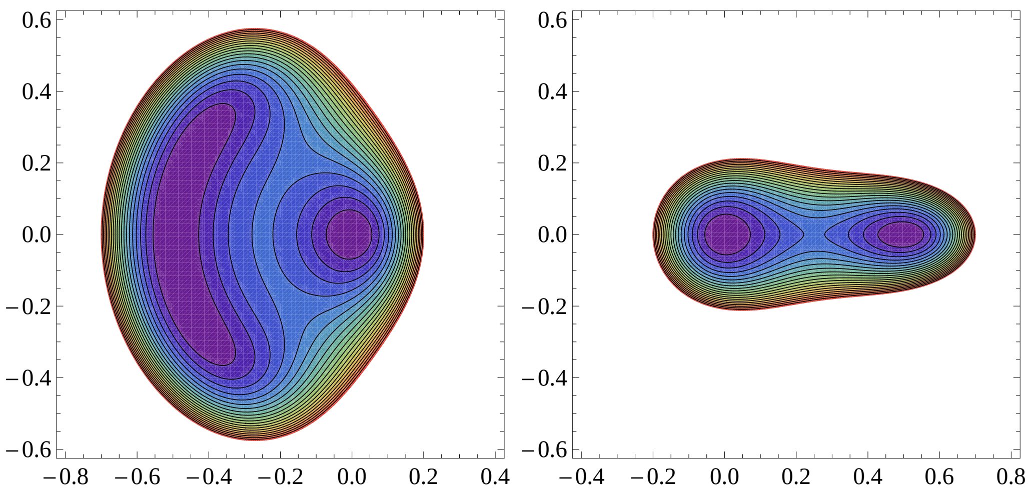
1.2 Function $f(\gamma)$

1.2.1 Choice 1

$$f_r^{(1)}(\gamma) = 2\left(\frac{\cos\gamma + 1}{2}\right)^r - 1 \tag{8}$$



(a) Function $f_r^{(1)}(\gamma)$ for $r = 1, 2, \ldots, 10$.



(b) γ-soft case for $r = 3$.

(c) γ-rigid case for $r = 3$.

Figure 1: Potential for Choice 1 of the γ dependence.

Function $f_r^{(1)}$ and the potential $\bar{V}$ are shown in Fig. 1. If $r > 1$, function $f_r^{(1)}$ makes the potential V γ-soft with the deformed minimum at $\gamma = \pi$. A γ-rigid case is obtained simply by taking the opposite function $-f_r^{(1)}$, which can effectively be done by the transformation $B \to -B$. In this case the deformed minimum sits at $\gamma = 0$.

r		1	$\cos\gamma$	$\cos 2\gamma$	$\cos 3\gamma$	$\cos 4\gamma$	$\cos 5\gamma$	$\cos 6\gamma$	$\cos 7\gamma$
1	1		1						
2	$\frac{1}{4}$	-1	4	1					
3	$\frac{1}{16}$	-6	15	6	1				
4	$\frac{1}{64}$	-29	56	28	8	1			
5	$\frac{1}{256}$	-130	210	120	45	10	1		
6	$\frac{1}{1024}$	-562	792	495	220	66	12	1	
7	$\frac{1}{4096}$	-2380	3003	2002	1001	364	91	14	1

Table 1: Explicit expressions for the first 7 functions $f_r^{(1)}(\gamma)$ with integer r. An example how to read in the table: $f_2^{(1)} = 1/4(-1 + 4\cos\gamma + \cos 2\gamma)$.

Table 1 gives the explicit expressions for a few of the lowest integer values of r.

A disadvantage of the function (8) is that in the soft case for integer $r >= 2$, it does not have the quadratic term in the Taylor series at the minimum (instead the minimum is approximated by a quartic function or a function of even higher order). In the rigid case, however, the quadratic term in the expansion exists and the potential (1) in the γ direction can be aproximated as

$$\bar{V}^{(1)\mathrm{rigid}}(\gamma) = \frac{A^2}{C} r\gamma^2 + O(\gamma)^3. \tag{9}$$

Hence the frequency of small γ vibrations is

$$\bar{\Omega}_\gamma^{(1)\mathrm{rigid}} = \sqrt{\frac{2A^2}{CK\bar{\beta}_2^2} r} = \sqrt{\frac{2A}{K} r} \tag{10}$$

and the rigidity ratio

$$\bar{R}^{(1)\mathrm{rigid}} = \sqrt{r} \tag{11}$$

(it is displayed in Fig. 2).

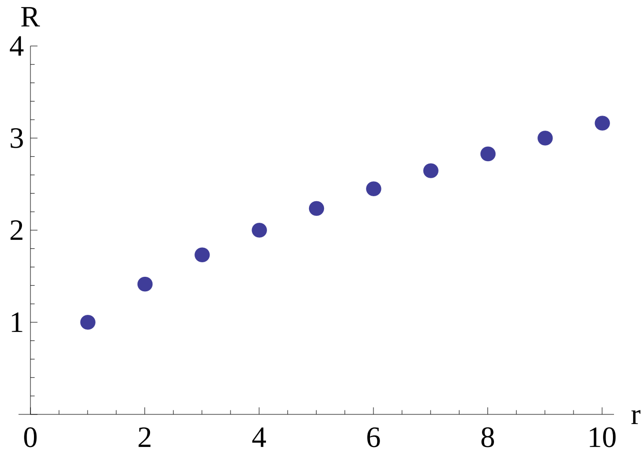
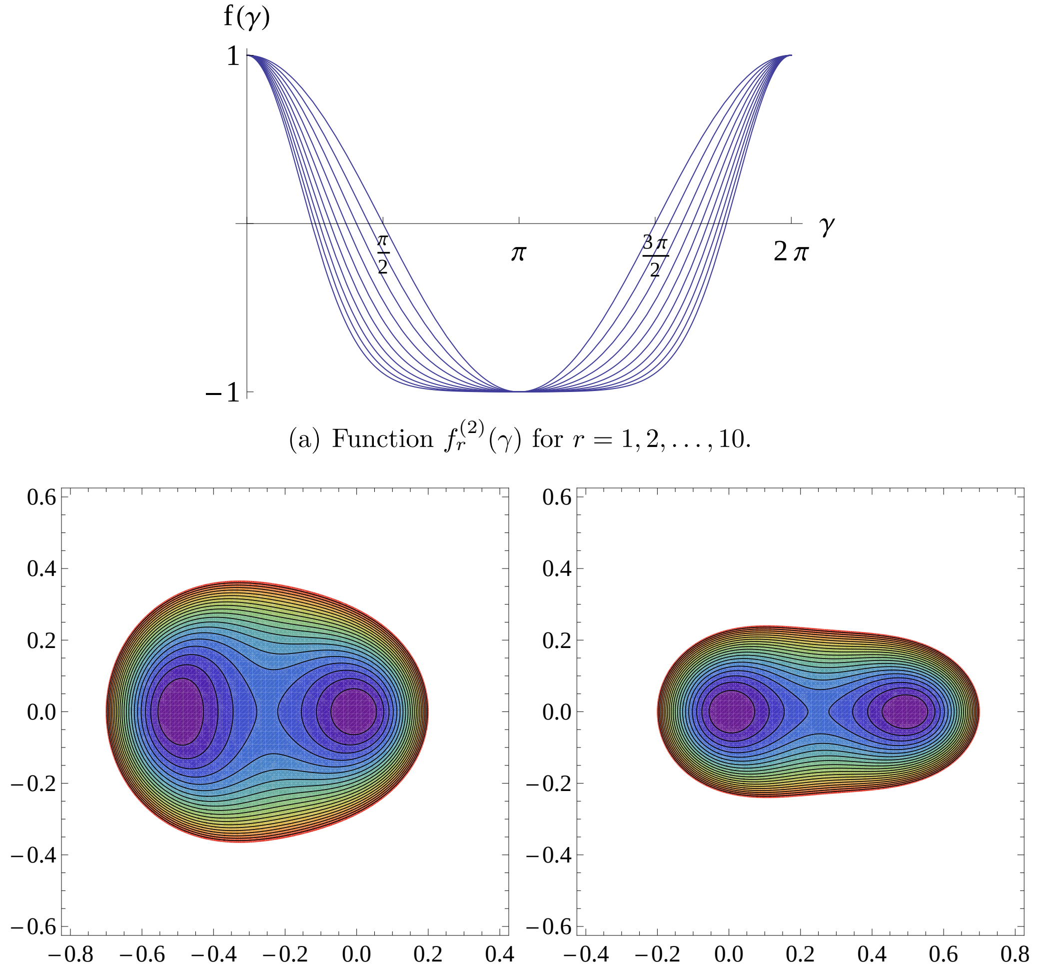


Figure 2: Rigidity ratio for integer r in the rigid case (Choice 1).

1.3 Choice 2

$$f_r^{(2)}(\gamma) = \frac{2}{2^r - 1}\left[\left(\frac{\cos\gamma + 3}{2}\right)^r - 1\right] - 1 \tag{12}$$



(a) Function $f_r^{(2)}(\gamma)$ for $r = 1, 2, \ldots, 10$.

(b) γ-soft case for $r = 3$.

(c) γ-rigid case for $r = 3$.

Figure 3: Potential for Choice 2 of the γ dependence.

Function $f_r^{(1)}$ and the potential $\bar{V}$ are shown in Fig. 1. If $r > 1$, function $f_r^{(1)}$ makes the potential V γ-soft with the deformed minimum at $\gamma = \pi$. A γ-rigid case is obtained simply by taking the opposite function $-f_r^{(1)}$, which can effectively be done by the transformation $B \to -B$. In this case the deformed minimum sits at $\gamma = 0$.

Table 1 gives the explicit expressions for a few of the lowest integer values of r.

Function $f_r^{(2)}$ and the potential $\bar{V}$ are shown in Fig. 3. Table 2 gives the explicit expressions for the lowest integer values of r.

The function covers again both γ-soft and -rigid cases in the same manner as is described in the previous Subsection. Its expansion in the deformed minimum has the quadratic term

r		1	$\cos\gamma$	$\cos 2\gamma$	$\cos 3\gamma$	$\cos 4\gamma$	$\cos 5\gamma$	$\cos 6\gamma$	$\cos 7\gamma$
1	1		1						
2	$\frac{1}{12}$	-1	12	1					
3	$\frac{1}{112}$	-18	111	18	1				
4	$\frac{1}{960}$	-221	936	220	24	1			
5	$\frac{1}{7936}$	-2310	7570	2280	365	30	1		
6	$\frac{1}{64512}$	-22162	59976	21615	4500	546	36	1	
7	$\frac{1}{520192}$	-202020	470267	194166	49161	7812	763	42	1

Table 2: Explicit expressions for the first 7 functions $f_r^{(2)}(\gamma)$ with integer r. An example how to read in the table: $f_2^{(1)} = 1/12(-1 + 12\cos\gamma + \cos 2\gamma)$.

in both cases: in the γ-soft case

$$\bar{V}^{(2)\text{soft}}(\gamma) = \frac{A^2}{C}\frac{r}{2^r - 1}(\gamma - \pi)^2 + O(\gamma - \pi)^3 \tag{13}$$

$$\bar{\Omega}_\gamma^{(2)\text{soft}} = \sqrt{\frac{2A}{K}\frac{r}{2^r - 1}} \tag{14}$$

$$\bar{R}^{(2)\text{soft}} = \sqrt{\frac{r}{2^r - 1}}, \tag{15}$$

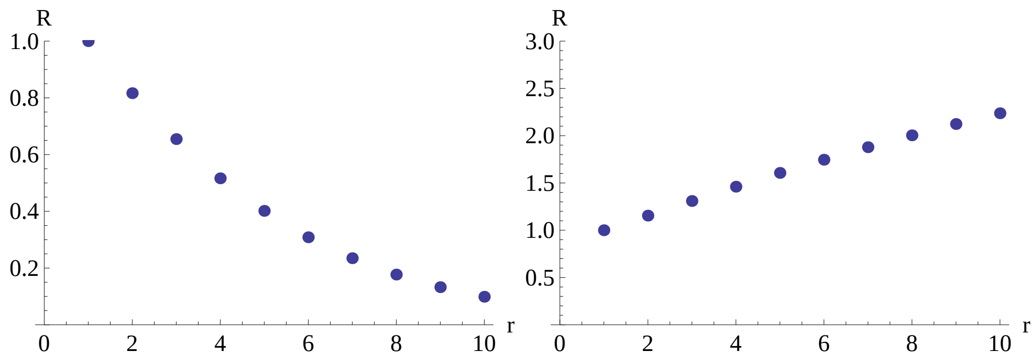
and the γ-rigid case

$$\bar{V}^{(2)\text{rigid}}(\gamma) = \frac{A^2}{C}\frac{r}{2}\frac{2^r}{2^r - 1}\gamma^2 + O(\gamma)^3 \tag{16}$$

$$\bar{\Omega}_\gamma^{(2)\text{rigid}} = \sqrt{\frac{2A}{K}\frac{r}{2}\frac{2^r}{2^r - 1}} \tag{17}$$

$$\bar{R}^{(2)\text{rigid}} = \sqrt{\frac{r}{2}\frac{2^r}{2^r - 1}}, \tag{18}$$

(displayed in Fig. 4).



(a) Soft case. (b) Rigid case.

Figure 4: Rigidity ratio for integer r (Choice 2).

1.4 Comments on the functions

1. Choice 2 gives smaller rigidity ratio in the rigid case.

2. If $r = 1$, which means $f(\gamma) = \cos\gamma$, then potential $\bar{V}$ is symmetric at the point of the barrier $\bar{\beta}_B$:

$$\begin{aligned}\bar{V} &= A\beta^2 + \sqrt{4AC}\beta^3\cos\gamma + C\beta^4 \\ &= A\beta^2 + \sqrt{4AC}\beta^2 x + C\beta^4 \\ &= A\left[\left(x' - \frac{1}{2}\sqrt{AC}\right)^2 + y^2\right]\left(A + \sqrt{4AC}\right) + C\left[\left(x' - \frac{1}{2}\sqrt{AC}\right)^2 + y^2\right]^2 \\ &= \frac{1}{16C}\left[A^2 + 8AC\left(-x'^2 + y^2\right) + 16C^2\left(x'^2 + y^2\right)^2\right] \end{aligned} \tag{19}$$

($x' = x - \bar{\beta}_B$) that is indeed even in both x' and y. The potential is plotted in Fig. 5.

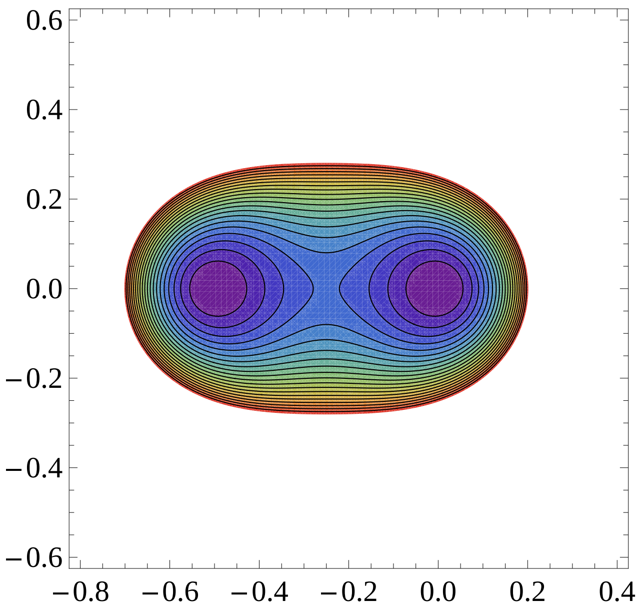


Figure 5: Demonstration of the symmetry of potential $\bar{V}$ with $f(\gamma) = \cos\gamma$ at the critical point.

3. The rigidity ratio R depends on the adjustable parameters A, B, C of the potential. It decreases for A below the critical point and diverges at the antispinodal point (where the deformed minimum disapears). An example is shown in Fig. 6.

1.5 Technical intermezzo: Diagonalization

1.5.1 Basis

The system is diagonalized in the basis

$$|nm\rangle = R_{nm}(\beta)\Phi_m(\gamma) \tag{20}$$

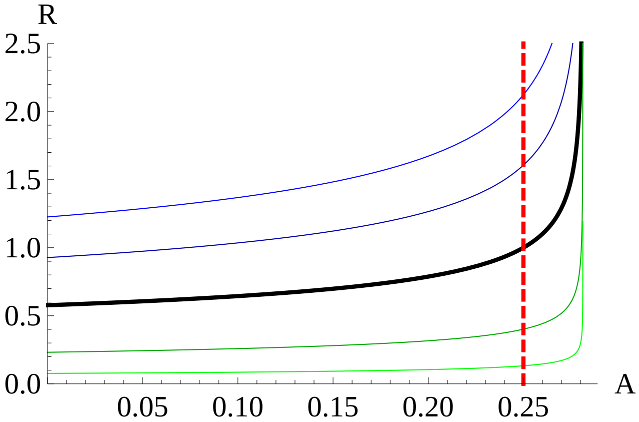


Figure 6: Dependence of the rigidity ratio R on parameter A for $C = 1$ and $f_r^{(2)}$ with $r = 1$ (black thick line), $r = 5, 9$ γ-soft (green lines below the black line), and $r = 5, 9$ γ-rigid (blue lines above the black line). The critical point is marked by the red dashed line.

of the 2D harmonic oscillator

$$H_0 = T + V_0 = -\frac{\hbar^2}{2K}\left(\frac{1}{\beta}\frac{\partial}{\partial\beta}\beta\frac{\partial}{\partial\beta} + \frac{1}{\beta^2}\frac{\partial^2}{\partial\gamma^2}\right) + A_0\beta^2. \tag{21}$$

where

$$R_{nm}(\beta) = \sqrt{\frac{2kn!}{(n+l)!}}\left(k\beta^2\right)^{l/2} \mathrm{e}^{-\frac{1}{2}k\beta^2} L_n^l\left(k\beta^2\right) \tag{22}$$

$$\Phi_m(\gamma) = \sqrt{\frac{1}{2\pi}} e^{\mathrm{i}m\gamma} \tag{23}$$

(L_n^l denotes a Laguerre polynomial, $l = |m|$ and $k = \sqrt{2A_0K/\hbar^2}$). The eigenvalues of (21) are

$$E_{nm}^{(0)} \equiv \langle nm|H_0|nm\rangle = \hbar\Omega(2n + l + 1), \tag{24}$$

where $\Omega = \sqrt{2A_0/K}$.

1.5.2 Matrix elements

The general expression for the matrix elements are [1]

$$\langle n', m+b|\beta^a \cos b\gamma|nm\rangle = \frac{1}{2}(1+\delta_{b0})\sqrt{\frac{n'!n!}{(n'+l')!(n+l)!}}\frac{(-1)^{n'+n+a}}{k^{a/2}}$$
$$\sum_s \frac{\left[\frac{1}{2}(a+l+l')+s\right]!\left[\frac{1}{2}(a-\Delta l)\right]!\left[\frac{1}{2}(a+\Delta l)\right]!}{s!(n'-s)!(n'+s)!\left[\frac{1}{2}(a-\Delta l)-n'+s\right]!\left[\frac{1}{2}(a+\Delta l)-n+s\right]!} \tag{25}$$

where

$$l = |m| \qquad l' = |m'| \qquad \Delta l = l' - l \tag{26}$$

and the limits of the summation are

$$\max\left\{0, n' - \frac{1}{2}(a-\Delta l), n - \frac{1}{2}(a+\Delta l)\right\} \leq s \leq \min\{n', n\} \qquad \text{for } a+b \text{ even,}$$
$$0 \leq s \leq \min\{n', n\} \qquad \text{for } a+b \text{ odd.} \tag{27}$$

It is possible to express the most frequently used matrix elements for the Hamiltonian (1) explicitly:

$$\langle nm|\beta^2|nm\rangle = \frac{1}{k}(2n+m+1) \tag{28}$$
$$\langle n+1, m|\beta^2|nm\rangle = -\frac{1}{k}\sqrt{(n+1)(n+m+1)} \tag{29}$$
$$\langle nm|\beta^4|nm\rangle = \frac{1}{k^2}[n(n-1)+(n+m+1)(5n+m+2)] \tag{30}$$
$$\langle n+1, m|\beta^4|nm\rangle = -\frac{2}{k^2}(2n+m+2)\sqrt{(n+m+1)(n+1)} \tag{31}$$
$$\langle n+2, m|\beta^4|nm\rangle = \frac{1}{k^2}\sqrt{(n+m+2)(n+m+1)(n+2)(n+1)} \tag{32}$$

The matrix elements of the term proportional to B must be calculated using the general formula (25).

If the indexes $i = \{n, m\}$

$$0 \leq n \leq N, -M \leq m \leq M, \tag{33}$$

of the Hamiltonian matrix are ordered in such a way that

$$\begin{aligned} &\ldots, i-1, i, i+1, \ldots, i+N, i+N+1 \ldots \\ &= \ldots, \{n-1, m\}, \{n, m\}, \{n+1, m\}, \ldots, \{n, m+1\}, \{n+1, m+1\}, \ldots \end{aligned} \tag{34}$$

(N, M limit the number of basis states), then the matrix has a band structure with

$$W = ([r]+1)\,N + 3(M \mod 2). \tag{35}$$

superdiagonals ($[\bullet]$ stands here for the nearest lower or equal even number).

1.5.3 Convergence

The convergence depends on the number of basis states given by N, M and on the basis stiffness A_0. The lower the Planck variable $\hbar$ is and the more the potential V differs from V_0, the more basis states are needed in order to achieve good convergence.

The system is diagonalized in the triangular basis whose states fulfill the condition

$$2n + |m| + 1 \leq \epsilon \tag{36}$$

[instead of the rectangular condition (33) given above]. Tables 3–6 give the best basis configurations for the systems that are studied in the following text. The error δ is defined as

$$\delta = \max_j \left\{ \frac{\left(E_j^{(\epsilon)} - E_0^{(\epsilon)}\right) - \left(E_j^{(\epsilon+10)} - E_0^{(\epsilon+10)}\right)}{E_j^{(\epsilon+10)} - E_0^{(\epsilon+10)}} \right\} \tag{37}$$

where $E_j^{(\epsilon)}$ is the j-th eigenvalue of the Hamiltonian matrix with the basis size limited by ϵ. The convergence criteria is assessed as $\delta \leq 1 \cdot 10^{-2}$.

A	A_0	ϵ	δ
0.5	0.3	50	$1.0 \cdot 10^{-4}$
0.4	0.18	60	$2.7 \cdot 10^{-6}$
0.3	0.08	70	$5.5 \cdot 10^{-4}$
0.25	0.06	80	$6.6 \cdot 10^{-3}$
0.2	0.06	100	$5.7 \cdot 10^{-3}$
0.15	0.07	120	$5.1 \cdot 10^{-3}$
0.1	0.07	140	$4.8 \cdot 10^{-3}$
0	0.07	160	$8.6 \cdot 10^{-3}$

Table 3: Basis parameters for f_1, $\hbar = 0.0015$, 500 well-converging states.

A	A_0	ϵ	δ
0.5	0.25	40	$5.8 \cdot 10^{-3}$
0.4	0.16	50	$1.0 \cdot 10^{-4}$
0.3	0.07	60	$6.4 \cdot 10^{-4}$
0.25	0.05	70	$3.9 \cdot 10^{-3}$
0.2	0.05	90	$3.1 \cdot 10^{-3}$
0.1	0.06	120	$4.1 \cdot 10^{-3}$
0	0.06	140	$4.0 \cdot 10^{-3}$

Table 4: Basis parameters for γ-soft $f_5^{(2)}$, $\hbar = 0.0015$, 500 well-converging states.

A	A_0	ϵ	δ
0.5	0.3	50	$1.2 \cdot 10^{-3}$
0.4	0.18	60	$1.8 \cdot 10^{-4}$
0.3	0.08	70	$5.1 \cdot 10^{-4}$
0.25	0.08	90	$1.4 \cdot 10^{-3}$
0.2	0.08	110	$4.7 \cdot 10^{-3}$
0.1	0.08	140	$1.0 \cdot 10^{-2}$
0	0.08	160	$1.0 \cdot 10^{-2}$

Table 5: Basis parameters for γ-rigid $f_5^{(2)}$, $\hbar = 0.0015$, 500 well-converging states.

A	A_0	ϵ	δ
0.5	0.25	40	$1.0 \cdot 10^{-3}$
0.4	0.16	45	$5.3 \cdot 10^{-4}$
0.3	0.06	50	$2.5 \cdot 10^{-3}$
0.25	0.04	65	$3.4 \cdot 10^{-3}$
0.2	0.05	80	$5.4 \cdot 10^{-3}$
0.1	0.05	100	$1.0 \cdot 10^{-2}$
0	0.05	110	$2.0 \cdot 10^{-3}$

Table 6: Basis parameters for γ-rigid $f_5^{(2)}$, $\hbar = 0.0015$, 500 well-converging states.

1.6 Results

I am calculating the level dynamics for Hamiltonan (1) with $f_r^{(2)}$ and the following values of the adjustable parameters:

$$
\begin{aligned}
B &= 1 \\
C &= 1 \\
\hbar &= 0.0015 \\
D &= 500
\end{aligned}
\tag{38}
$$

(D is the number of calculated eigenlevels). So far I have finished these cases:

1. The basic $r = 1$ case, $\bar{R} = 1$. The level dynamics is in Fig. 7. At the critical point $A = 1/4$, 13 states penetrate the barrier.

2. The γ-soft $r = 5$ case, $\bar{R} = \sqrt{\frac{5}{31}} \approx 0.40$, see Fig. 8. At the critical point 28 states pass through the barrier.

3. The γ-rigid $r = 5$ case, $\bar{R} = 4\sqrt{\frac{5}{31}} \approx 1.6$, see Fig. 9. At the critical point 10 states pass through the barrier.

4. The γ-soft $r = 9$ case, $\bar{R} = \frac{3}{\sqrt{511}} \approx 0.13$, see Fig. 10. At the critical point 50 states pass through the barrier.

References

[1] S. Bell, *J. Phys. B: Atom. Molec. Phys.* **3**, 745 (1970).

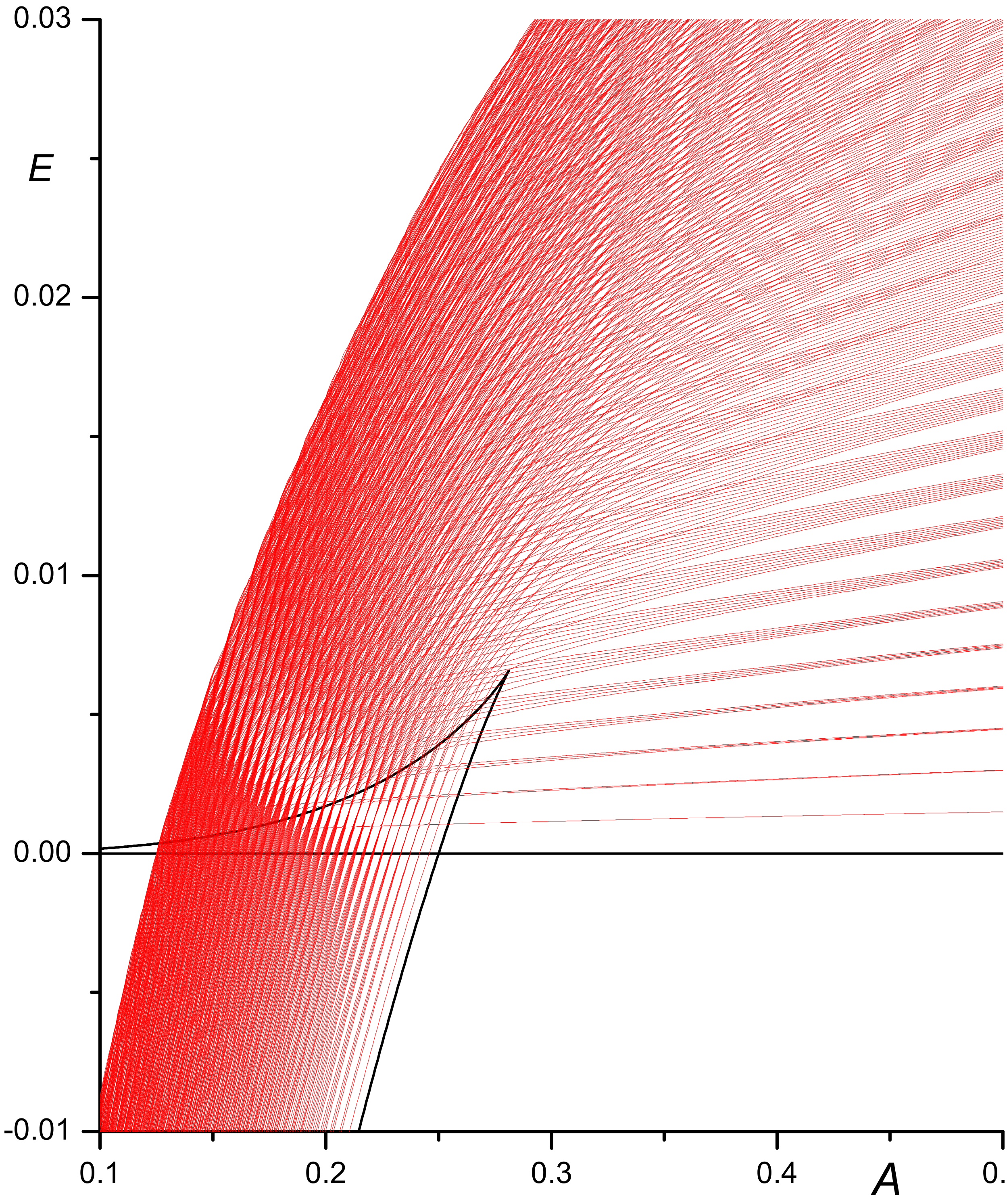


Figure 7: Level dynamics for the system with $f_1 = \cos\gamma$ angular dependence, $B = C = 1$, $\hbar = 500$, $D = 500$ displayed eigenstates. The calculation step is $\Delta A = 0.001$.

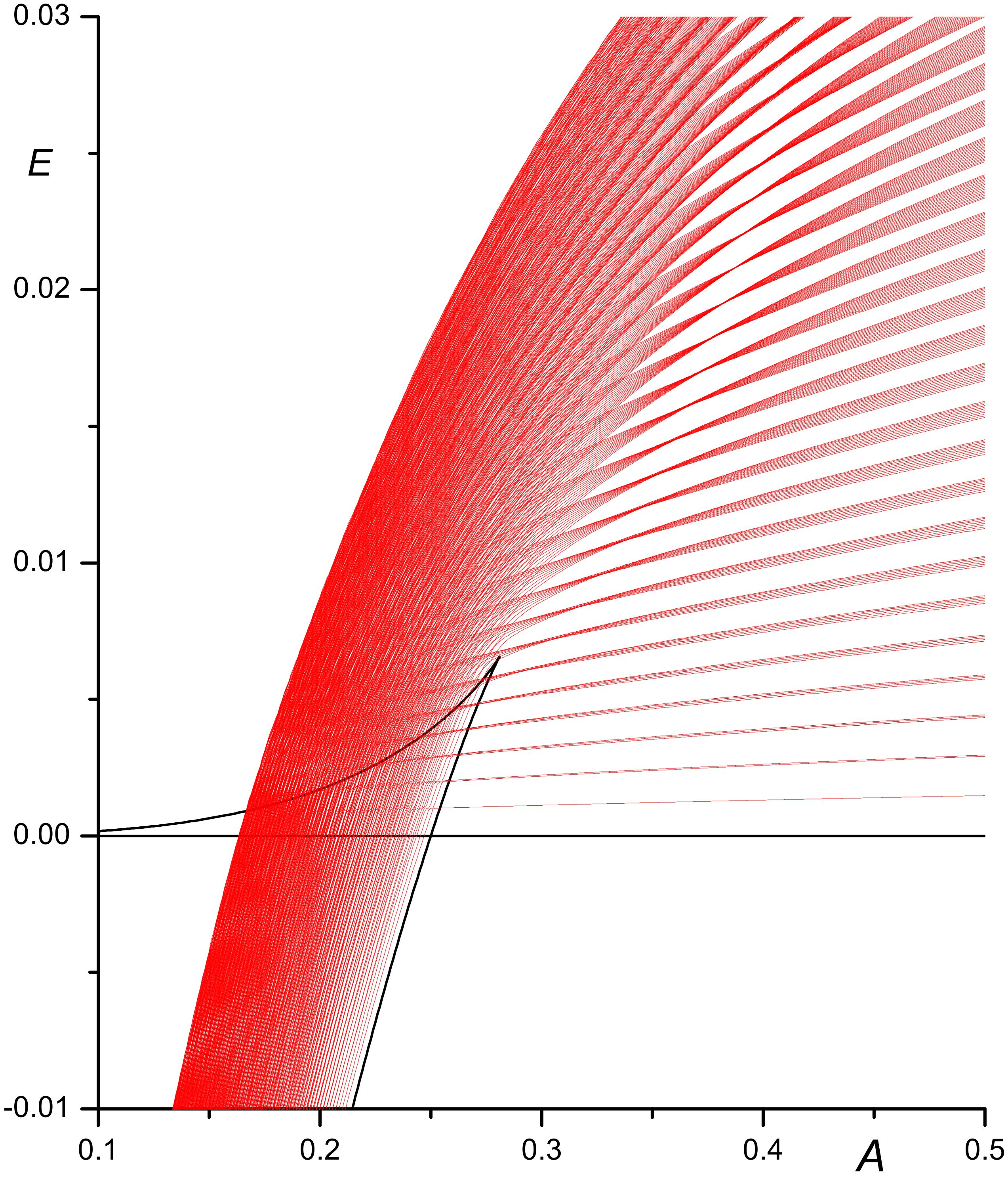


Figure 8: The same as in Fig.7, here for the γ-soft case $f_5^{(2)}$.

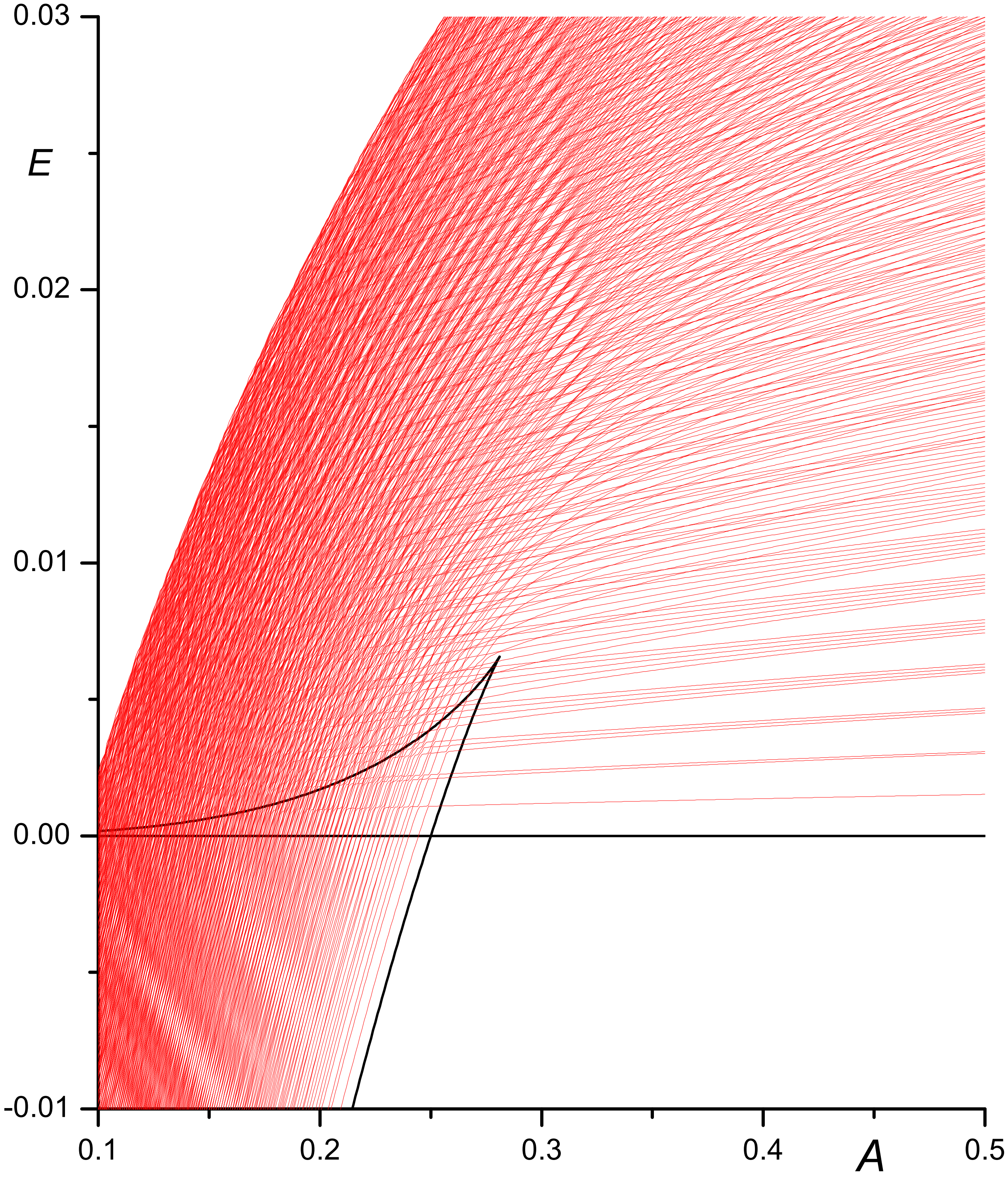


Figure 9: The same as in Fig.7, here for the γ-rigid case $f_5^{(2)}$.

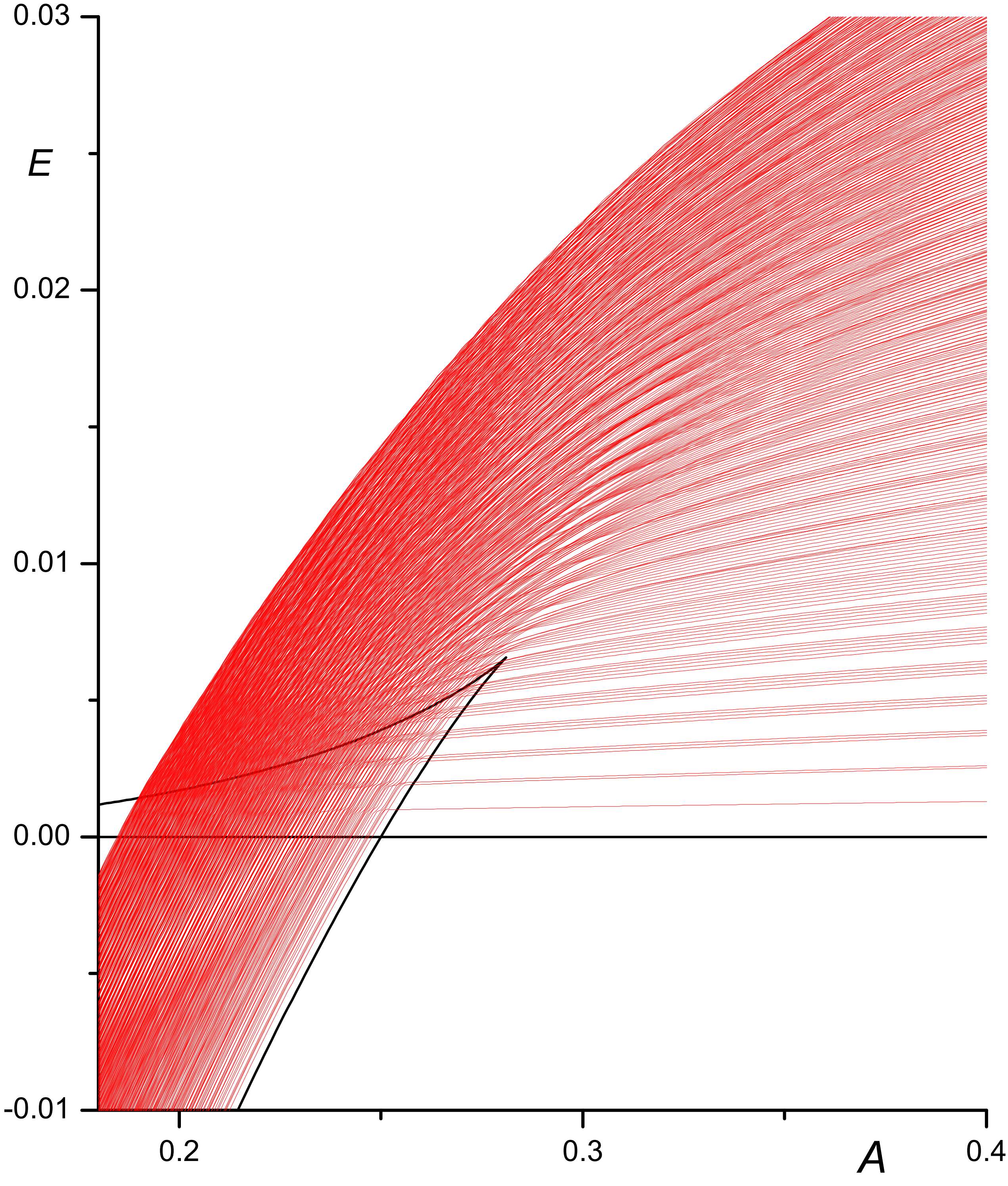


Figure 10: The same as in Fig.7, here for the γ-soft case $f_9^{(2)}$.