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We present an example of three-level non-adiabatic transition probability problem in which virtual turning points (or, active new Stokes curves) are inevitable for calculation of the transition probabilities.

The equation we consider is

$$i\frac{d}{dt}\Psi = \eta H(t,\eta)\Psi, \tag{1}$$

where $\Psi = \Psi(t,\eta)$ is a 3-vector, $\eta > 0$ is a large parameter and $H(t,\eta)$ is a 3×3 matrix given below:

$$\begin{aligned} H(t,\eta) &= H_0(t) + \eta^{-1/2}H_{1/2} \\ &= \begin{pmatrix} \rho_1(t) & 0 & 0 \\ 0 & \rho_2(t) & 0 \\ 0 & 0 & \rho_3(t) \end{pmatrix} + \eta^{-1/2}\begin{pmatrix} 0 & c_{12} & c_{13} \\ \overline{c_{12}} & 0 & c_{23} \\ \overline{c_{13}} & \overline{c_{23}} & 0 \end{pmatrix} \end{aligned} \tag{2}$$

with real polynomials $\rho_1(t)$, $\rho_2(t)$, $\rho_3(t)$ and complex constants c_{12}, c_{13}, c_{23}. Calculating transition probabilities is reduced to calculating continuation of solutions of (1) from $t = -\infty$ to $t = +\infty$. See [AKT2] and references cited there for detail.

In [AKT2], examples which have turning points only on the real axis are studied from the viewpoint of the exact WKB analysis, and in such cases new Stokes curves (, which were first discovered in [BNR]) are always inert near the real axis ([AKT2, §4]). Therefore virtual turning points (, which were introduced in [AKT1]) and new Stokes curves are irrelevant to the transition probabilities, that is, we obtain correct connection matrix by calculating analytic continuation along the real axis even if we ignore virtual turning points and new Stokes curves. Then in [S], a family of examples which have turning points off the real axis is considered, and there are active Stokes curves crossing the real axis. Thus, if we consider continuation along the real axis, we cannot disregard new Stokes curves. As a matter of fact, in those examples we can find paths from $t = -\infty$ to $t = +\infty$ which avoid all active parts of new Stokes curves. At the same time, the paths are very complicated and, in order to find out such paths, we need precise information about the location of new Stokes curves, as is mentioned in [S].

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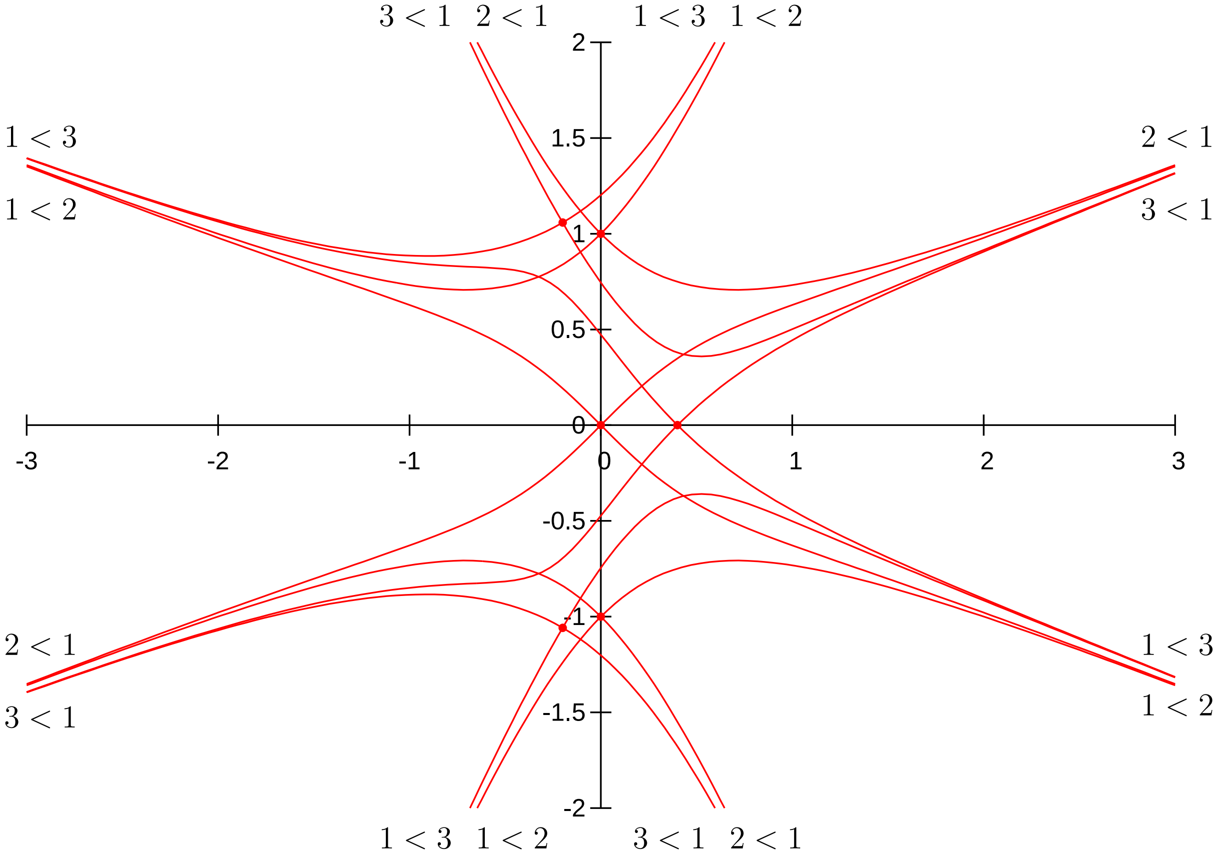

Figure 1: Turning points and ordinary Stokes curves for $c = 0.4$.

In this article, we present an example in which there is no path from $t = -\infty$ to $t = +\infty$ avoiding all active new Stokes curves, so that we have another evidence which manifests the importance of virtual turning points and new Stokes curves in this problem.

Let $\rho_1(t) = t^3$, $\rho_2(t) = -t$ and $\rho_3(t) = -t + c + c^3$ with $c = 0.4$. Then turning points of type $(1, 2)$ are at 0, $\pm i$ and those of type $(1, 3)$ are at 0.4, $-0.2 \pm i\sqrt{1.12}$. The configuration of its turninig points and Stokes curves is shown in Figure 1. Inequalities express types of Stokes curves. For example, $1 < 2$ means that $(\eta/i) \int_{t_0}^{t} (\rho_1 - \rho_2)\, dt < 0$ holds on the curve, where t_0 is the turning point from which the curve emanates.

Now in order to obtain complete Stokes geometry we add virtual turning points and new Stokes curves accoding to the procedure explained in [AKT2]. Here a complete Stokes geometry means a collection of (ordinary and virtual) turning points and Stokes curves emanating from them in which all the ordered crossing points of Stokes curves are resolved. (Cf. [AKT2].) Actually we encounter some degeneracy of Stokes geometry in the process, and so we give small perturbation $c = 0.4 \mapsto 0.4 + 0.01i$. Then the procedure gives the Stokes geometry shown in Figure 2. Blue dots represent virtual turning points, blue lines are new Stokes curves, whose dashed (resp. solid) parts are inert (resp. active). Neighborhoods of $t = -0.05 + i$, -0.1 and $-0.175 - 1.05i$ are enlarged. We find that there is a 'barrier' of active new Stokes curves and that we cannot go from $t = -\infty$ to $t = +\infty$ without crossing an active new Stokes curve. In order to make it easy to grasp the situation, we present Figure 3, where ordinary Stokes curves, i.e., red curves are presented by dashed lines. We emphasize that a barrier is also formed solely by Stokes

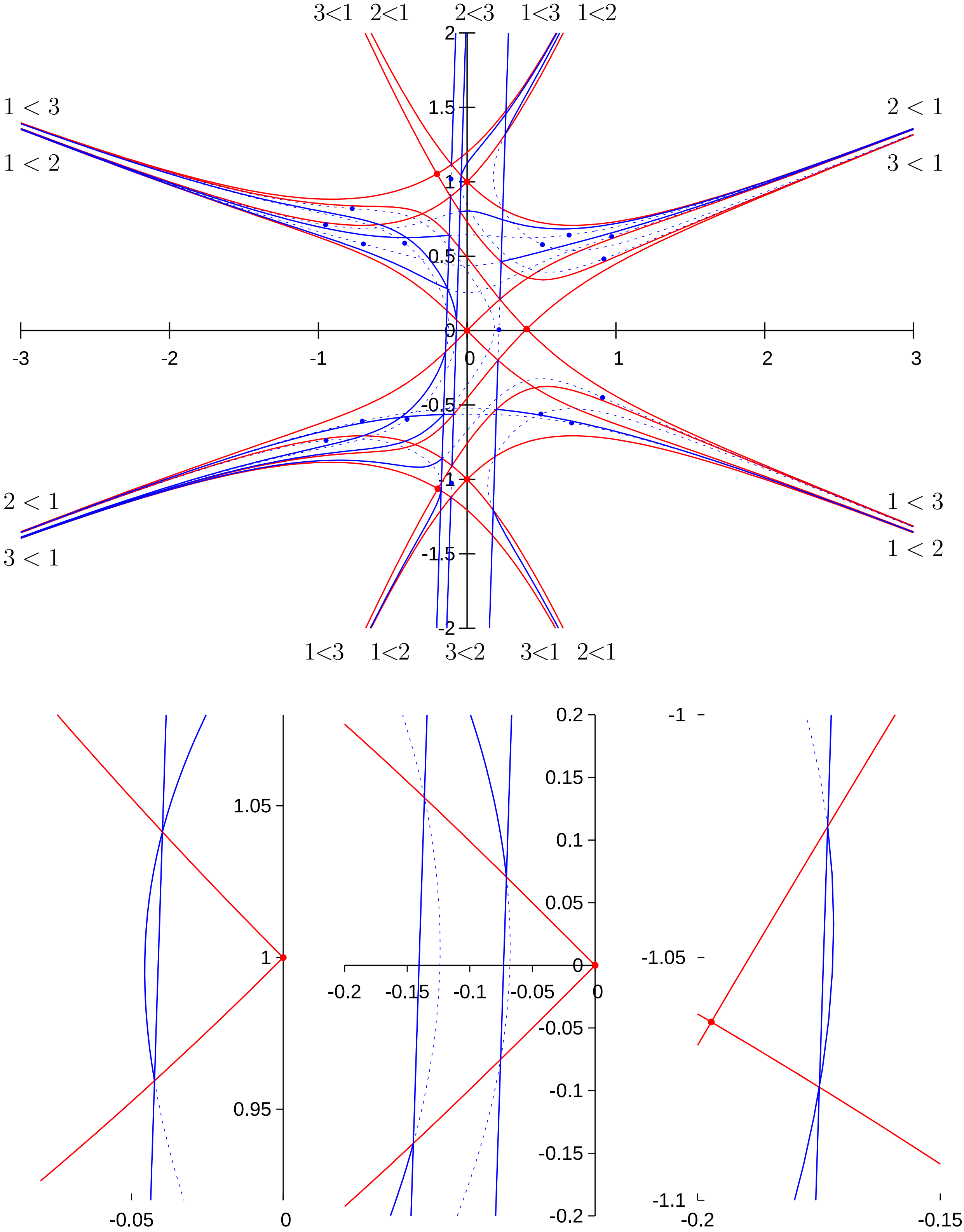

Figure 2: Complete Stokes geometry for $c = 0.4 + 0.01i$. Some parts near the imaginary axis are enlarged.

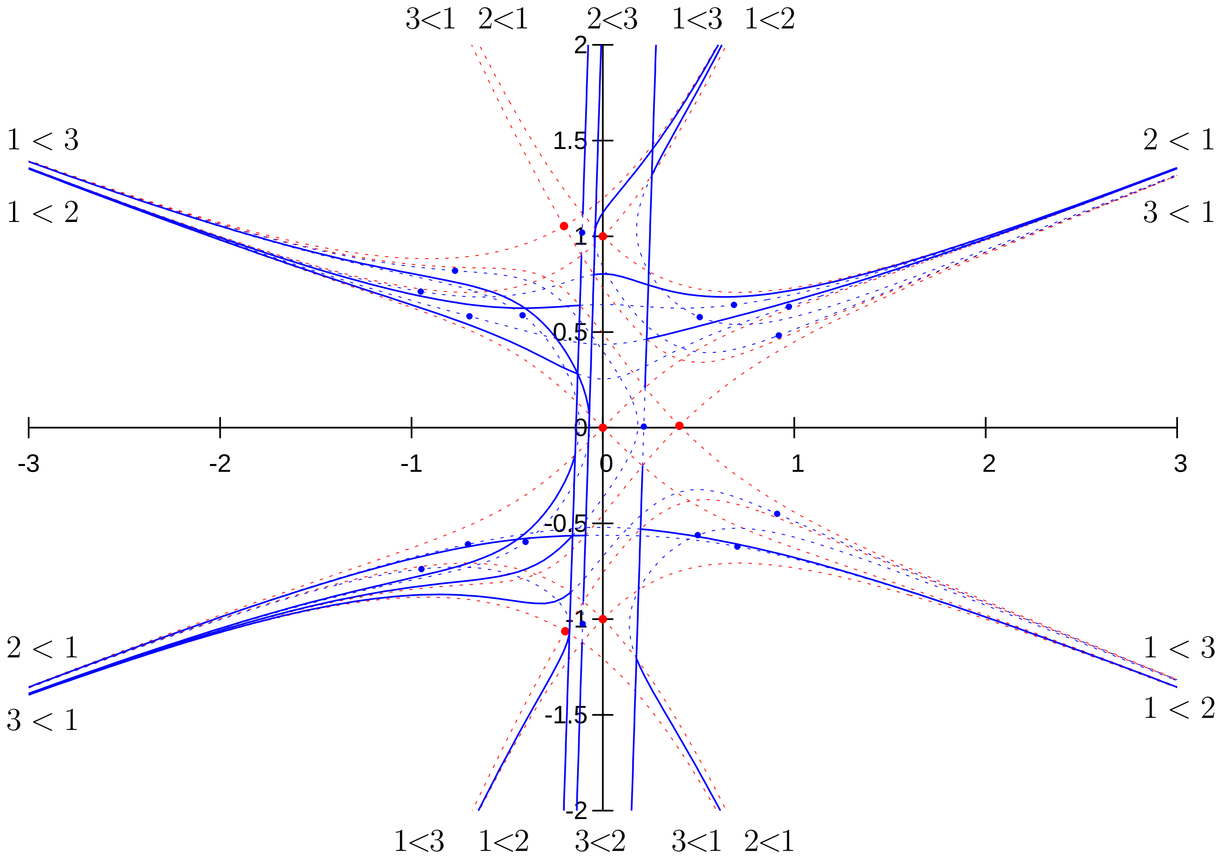

Figure 3: ‘Barrier’ of active Stokes curves for $c = 0.4 + 0.01i$.

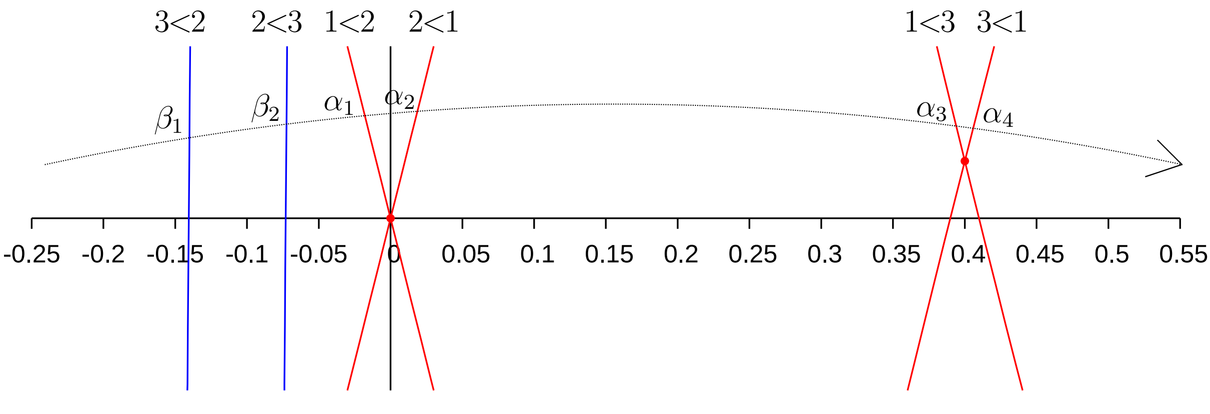

Figure 4: Stokes curves near the real axis for $c = 0.4 + 0.01i$. Inert new Stokes curves are omitted.

curves on which WKB solutions of type 2 is dominant (i.e., the label "$1 < 2$" or "$3 < 2$" is attached to them). Therefore as we calculate the analytic continuation of solutions of (1), it is inevitable to go across an active new Stokes curve.

Now apart from the problem whether we can avoid active new Stokes curves or not, we carry out the calculation of analytic continuation from $t = -\infty$ to $t = +\infty$ along the real axis. First, let us check the configuration of active (ordinary and new) Stokes curves near the real axis. There are eight ordinary Stokes curves and two new Stokes curves (Figure 4). To describe the continuation concretely, let $\Psi^{(j)}$ be a WKB solution of type j (namely a WKB solution whose exponential factor is $\exp[(\eta/i)\int_{t_0}^{t}\rho_j(t)\,dt]$) ($j = 1, 2, 3$). See [AKT2] for details about WKB solutions of (1). We avoid the two turning points upward, and encounter two new Stokes curves and four ordinary ones (Figure 4). Then we let α_1, α_2, α_3, α_4, β_1 and β_2 denote the Stokes coefficients for those Stokes curves as specified in Figure 4. For example, when we pass over the Stokes curve to which β_1 is attached, WKB solutions change as $(\Psi^{(1)}, \Psi^{(2)}, \Psi^{(3)}) \mapsto (\Psi^{(1)}, \Psi^{(2)} + \beta_1\Psi^{(3)}, \Psi^{(3)})$. Combining six relations of this kind together, we then obtain

$$(\Psi^{(1)}, \Psi^{(2)}, \Psi^{(3)}) \mapsto (\Psi^{(1)}, \Psi^{(2)}, \Psi^{(3)})M_+ \tag{3}$$

with the connection matrix

$$M_+ = \begin{pmatrix} 1 & \alpha_1(1+\beta_1\beta_2)+\alpha_3\beta_1 & \alpha_3+\alpha_1\beta_2 \\ \alpha_2 & (1+\alpha_1\alpha_2)(1+\beta_1\beta_2) & (1+\alpha_1\alpha_2)\beta_2 \\ \alpha_4 & \alpha_1\alpha_4(1+\beta_1\beta_2)+(1+\alpha_3\alpha_4)\beta_1 & 1+\alpha_3\alpha_4+\alpha_1\alpha_4\beta_2 \end{pmatrix}. \tag{4}$$

Noting that (j, k)-element is related to the probability of transition from k to j (if we take suitably normalized WKB solutions as $\Psi^{(j)}$'s), we look at $(2, 3)$-element $(1+\alpha_1\alpha_2)\beta_2$, which is proportional to β_2. Recalling that β_2 is a Stokes coefficient attached to a new Stokes curve, we conclude that the effect of virtual turning points and new Stokes curves is inevitable for calculationg transition probabilities of this example.

Now we give a few remarks on this transition. The new Stokes curve to which β_2 is attached originates from a virtual turning point in the lower half-plane ($\simeq -0.105724 - 1.024767i$), and it passes through ordered crossing points of Stokes curves emanating from the couple of turning points thereabout. In Figure 5 we focus our attention on the configuration of the new Stokes curve mentioned above together with ordinary Stokes curves relevant to it; some other Stokes curves are omitted for the simplicity of illustration. In Figure 5 the crossing point C of the ordinary Stokes curves emanating from t_j ($j = 1, 2$) to which Stokes coefficient α_5 and α_6 are attached, is an ordered one, and it is resolved by the new Stokes curve emanationg from the virtual turning point v; it is inert near v, and after passing over the crossing point, it becomes active with the Stokes coefficient β_2, which is actually

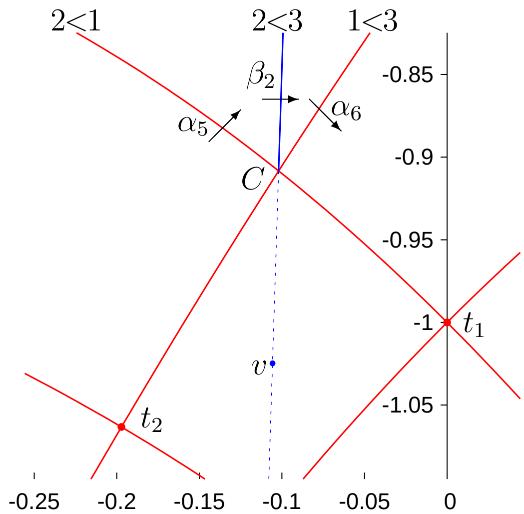

Figure 5: Configuration of some Stokes curves near a virtual turning point in the lower half-plane.

given by $\alpha_5\alpha_6$. (See, e.g., [BNR], [AKT1].) At the same time, any Stokes curve from t_j ($j = 1, 2$) does not cross the real axis. Therefore we have found that the new Stokes curve in question visualizes the indirect effect of t_1 and t_2 to the transition probabilities.

As for quantitative features of Stokes coefficients, some exponential factors are contained in them. More specifically, for a Stokes curve of type $j < k$ emanating from a turning point t_{jk}, $\exp[(\eta/i)\int_{t_0}^{t_{jk}}(\rho_k - \rho_j)\,dt]$ is included in the Stokes coefficient, where t_0 is a point on the real axis (cf. [AKT2, §4]). Therefore Stokes coefficients related to turning points on the real axis such as α_1, α_2, α_3 and α_4 are not exponentially large nor small. On the other hand, β_2 is exponentially small. In fact, since $\beta_2 = \alpha_5\alpha_6$ holds, its exponential factor can be written as

$$\exp\left[\frac{\eta}{i}\int_{t_0}^{C}(\rho_3 - \rho_2)\,dt + \frac{\eta}{i}\int_{C}^{t_1}(\rho_1 - \rho_2)\,dt + \frac{\eta}{i}\int_{C}^{t_2}(\rho_3 - \rho_1)\,dt\right], \tag{5}$$

each term of whose exponent is negative. Similarly β_1 is also exponentially small. Thus most of terms in M_+ having β_1 or β_2 could be negligible in that they are exponentially small compared to the other terms. Still, as to $(2, 3)$-element, such terms give the only contribution, and we cannot disregard at all.

As ending this article, we give some materials for the opposite perturbation $c = 0.4 \mapsto 0.4-0.01i$. Figure 6 is the complete Stokes geometry. Neighborhoods of $t = -0.175+1.05i$, -0.1 and $-0.05 - i$ are enlarged. Red lines are dashed in Figure 7. Figure 8 shows the configuration near the real axis. We remark that the location of the two new Stokes curves is reversed. The connection matrix is

$$M_- = \begin{pmatrix} 1 & \alpha_1 + \alpha_3\beta_1 & \alpha_3(1 + \beta_1\beta_2) + \alpha_1\beta_2 \\ \alpha_2 & 1 + \alpha_1\alpha_2 & (1 + \alpha_1\alpha_2)\beta_2 \\ \alpha_4 & \alpha_1\alpha_4 + (1 + \alpha_3\alpha_4)\beta_1 & (1 + \alpha_3\alpha_4)(1 + \beta_1\beta_2) + \alpha_1\alpha_4\beta_2 \end{pmatrix}. \tag{6}$$

Concerning this perturbation, we reach the same conclusion.

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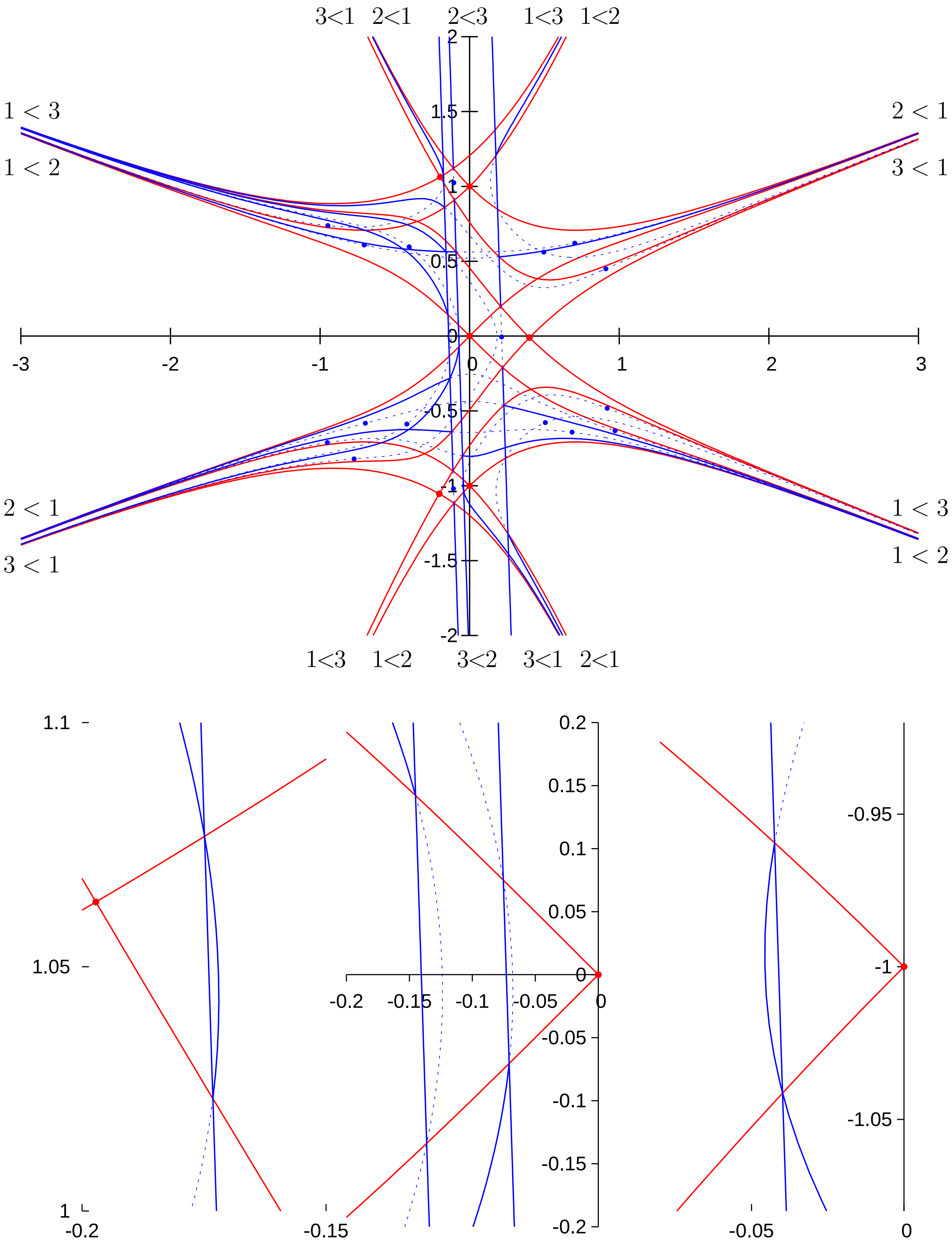

Figure 6: Complete Stokes geometry for $c = 0.4 - 0.01i$. Some parts near the imaginary axis are enlarged.

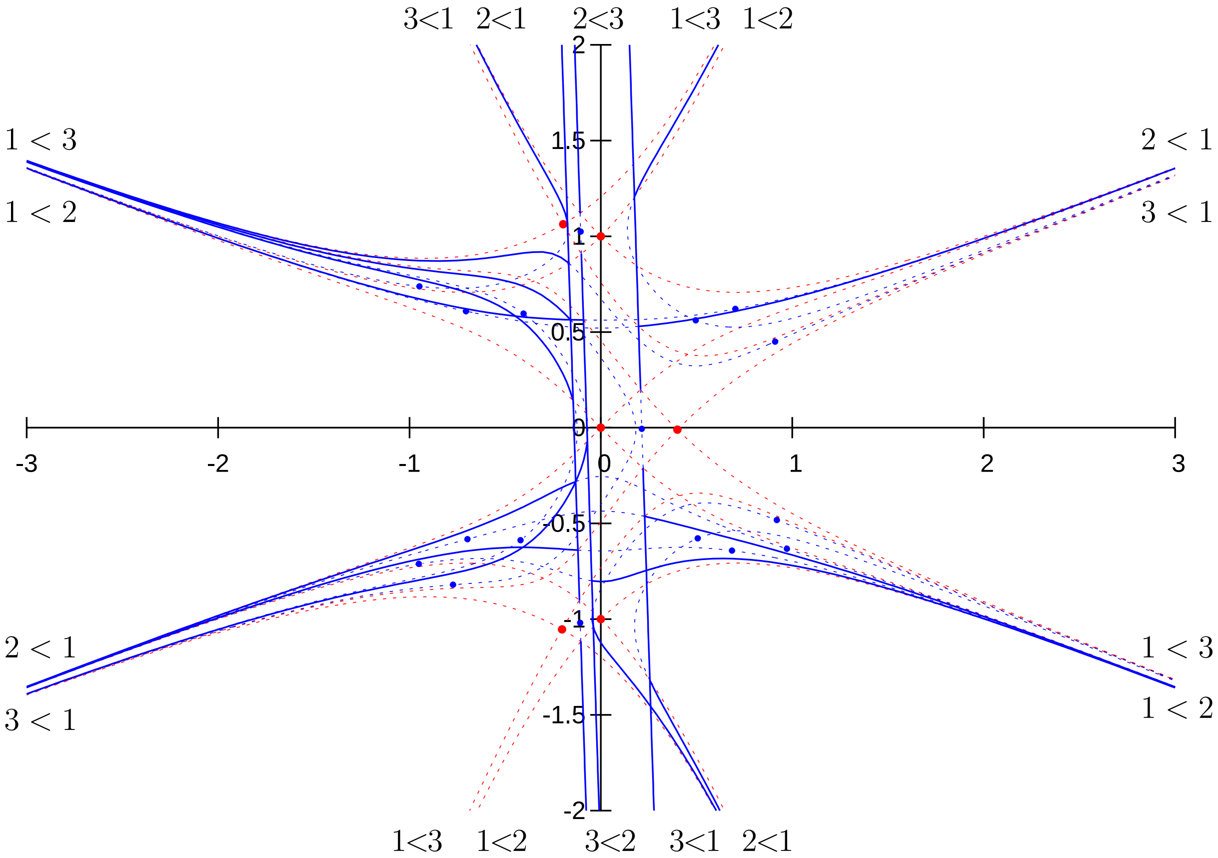

Figure 7: 'Barrier' of active Stokes curves for $c = 0.4 - 0.01i$.

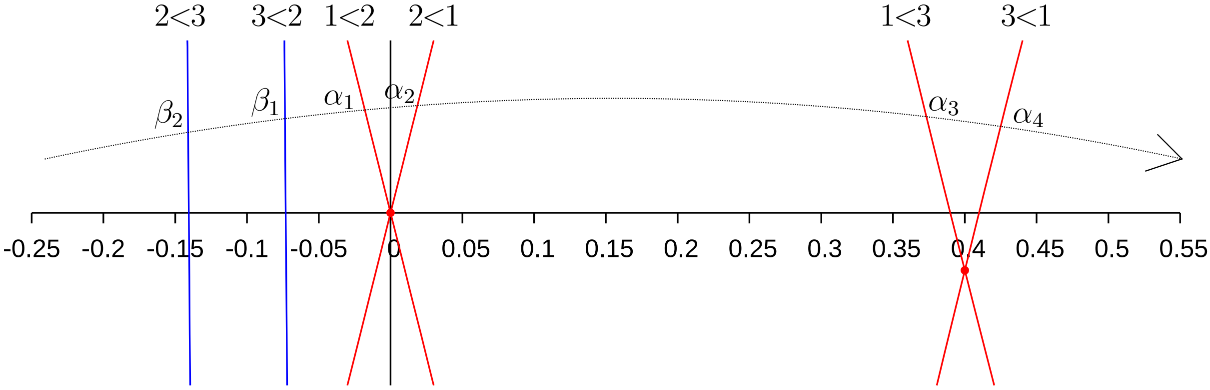

Figure 8: Stokes curves near the real axis for $c = 0.4 - 0.01i$. Inert new Stokes curves are omitted.