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Abstract

The unavoidability of metastable behaviour in digital circuit-components like flip-flops, arbiters and synchronisers is based on the assumption that the point representing such systems in phase space follows a trajectory which depends continuously on initial conditions. The validity of this assumption is well-established for existing implementations, and claimed for all implementations that are possible according to the classical laws of physics. In this paper we argue that the validity of the continuity assumption for quantum mechanical systems is an open question.

Contents

1 Introduction

Metastable behaviour occurs in digital circuits when the voltage level in some part of the circuit remains undefined for an indefinite period of time. During this time the voltage level is somewhere in between the ranges corresponding to the logical 1- and 0-values. These ranges form so called stable states of a flip-flop or any other bistable digital circuit, i.e. an external force is needed to drive the system from a high voltage value (corresponding to a logical 1) to a low voltage value (corresponding to a logical 0) or vice versa, but internal forces (like thermal fluctuations of the atoms and electrons) cannot achieve this.

When a bistable system is driven from one stable state to another, its corresponding point in phase space crosses a region of indecision where it can stay forever if the driving force is switched off instantaneously after entering this region, until noise causes the system to leave the region of indecision. Outside this region the phase point will move to one of the stable states and stay there as long as the driving force remains switched off. One may argue that the probability that the driving force is switched off exactly at the moment that the phase point enters the region of indecision is zero, but if it is switched off a little later or earlier, the time that the phase point needs to reach one of the stable states will become infinite (in the absence of noise) when this deviation in switch-off time approaches zero. There is thus a finite probability that the voltage level remains undefined for an arbitrary finite period of time after the external driving force has been switched off. This is due to the fact that the phase point's position in phase space depends continuously on time and on its initial position. So if the driving force is switched off a little later or earlier, the phase point's initial position is close to the region of indecision and must therefore remain close to that region for a time which becomes longer the closer the initial position was to the region of indecision. We say that a bistable system has metastable behaviour if the time needed to reach one of the stable states is unbounded or infinite when the driving force is zero.

Actually, the continuous dependence of the phase point's position on time and initial position is a fundamental assumption. No proof from first principles is known, but it is generally accepted by most physicists for all physical systems whose evolution in time can be represented by a phase point's trajectory in phase space. Also when one looks in an arbitrary textbook on ordinary differential equations, the first theorems one finds are on existence and uniqueness of solutions and on their continuous dependence on initial conditions. This is closely related to the well-posedness criterion in mathematical physics: if a system is modelled by a set of differential equations which does not have a unique solution that depends continuously on initial (or boundary) conditions, it is said that the problem is not well-posed.

The formal proof that this well-posedness criterion makes metastable behaviour in digital systems unavoidable was first given by Hurtado [Hur75] and subsequently generalised by Marino [Mar81] and by Kleeman and Cantoni [KC87]. The question remains however, whether this well-posedness criterion is indeed universally valid for all physical systems, as claimed by Marino. If this criterion applies and the region of indecision has an equilibrium point, it follows that this point cannot be reached in a finite time (in the absence of noise),

because other trajectories outside this region will eventually approach one of the stable states. This asymptotical approach of an unstable equilibrium point is well known in the description of phase transitions in physical systems at their critical point as *critical slowing down*. During the last decade (external) noise induced transitions have drawn much attention from physicists. Such transitions are described by so called stochastic differential equations, for which the meaning of the well-posedness criterion is entirely different. The switching of an optical gate forms an interesting example of such a noise induced transition. Horsthemke [HL84] describes a large class of these transitions that all exhibit critical slowing down. He also mentions a notable exception: the Verhulst model. In this model one of the boundaries of the state space coincides with an equilibrium point. Furthermore, in 1986 Doering proved that the stochastic Landau equation does not exhibit critical slowing down [Doe86]. Unfortunately this does not apply to the switching of an optical gate, so the optical digital circuits under development now will also show metastable behaviour. Nevertheless, the critical slowing down can be compensated in part by the application of noise as described by Lugiato et al. [LBMP89]. Whether it can be completely avoided in an as yet unknown new type of optical gate based on the Verhulst model or the stochastic Landau equation, is an open question.

In this paper we don't investigate this question any further. Our main objective is to show what type of violation of the well-posedness criterion is sufficient to avoid metastable behaviour and to discuss its physical plausibility. The formal proof by Hurtado will not be repeated here, but illustrated by a stepwise transformation of a digital circuit implementation with metastable behaviour into one without metastable behaviour. Of course after each step the implementations become more abstract, since concrete implementations without metastable behaviour are not known. At the same time this transformation provides a motivation for the type of violation of the well-posedness criterion we finally arrive at.

First we describe a concrete digital circuit displaying metastable behaviour. Then we show how threshold voltages of transistors should be modified in order to avoid metastable behaviour. Then we show that also the relation between voltage and current of a transistor in its saturated state should be modified. After that we show that application of the well-posedness criterion implies the elimination of the metastable point from phase space, but not the elimination of metastable behaviour. This is because trajectories on different sides of the region of indecision (a line in our case) do not diverge into different regions of phase space, so that the system cannot resolve to one stable state or the other. Subsequently we show how this deficiency can be remedied by changing a parameter in the model. Metastable behaviour is still not eliminated, however, on account of the continuous dependence of a phase point's trajectory on initial conditions. Next we argue that branching of the former region of indecision into two different trajectories, each going to a different stable state, is sufficient to eliminate metastable behaviour, if the continuity assumption is relaxed to what we call semicontinuity. We then give a very simplified model of a flip-flop, where the stable states are holes separated by a hill. A transition takes place when a ball rolls from one hole over the hill to the other one. Metastable behaviour is characterised by the ball staying on top of the hill. We show how for certain shapes of the

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hill metastable behaviour can be eliminated if semicontinuity is assumed. Whether such hill shapes actually exist in nature, is of course the big question. We briefly discuss a recent article from the physics literature (about "terminal chaos") that affirms this hypothesis, but do not speculate on its plausibility. Finally we discuss some possibilities of bistable quantum mechanical systems without metastable behaviour, using the quantum potential approach. To date only numerical evidence for branching trajectories exists, however. We therefore conclude that the claim of Marino, Kleeman, Cantoni and others that no physical bistable system without metastable behaviour can exist is unwarranted, and should rather be considered as an open question.

2   The mousetrap

We start with a simple digital circuit displaying metastable behaviour. It consists of two p- and three n-transistors. One of the n-transistors can be used to drive the circuit from one stable state to the other. Initially the voltage at point X is high and at point W low (see
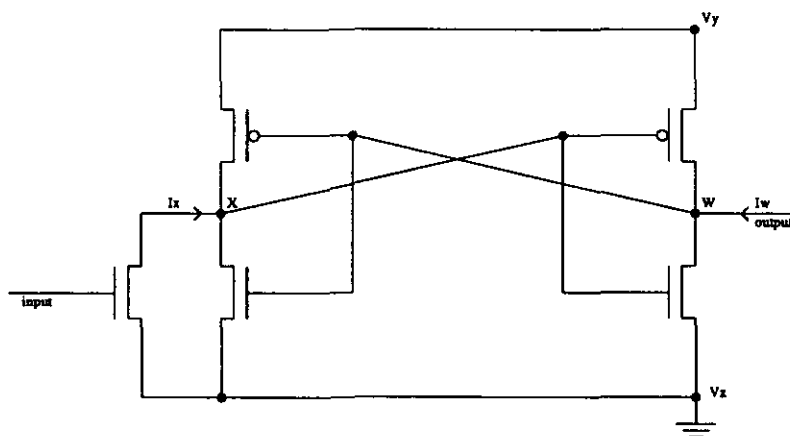

Figure 1: The mousetrap circuit.

fig.1). Also the gate-voltage of the drive-transistor is initially low. If this voltage becomes high then after some time the voltage at point X becomes low and at point W high. After X and W have become stable it doesn't matter anymore whether the drive-transistor's gate-voltage remains high or becomes low again. If it becomes low again before X and W have stabilised two things can happen depending on the time that the drive-transistor's gate-voltage remains high. If this voltage remains high only for a short period then X becomes high again and W low. If on the other hand the gate-voltage remains high long enough then X becomes low and W high. So the circuit can only make a single transition from one stable state to the other, hence its name "mousetrap" (due to Charles E. Molnar who did much pioneering work in the exploration of metastable behaviour in digital circuits). We are particularly interested in the case where the gate-voltage remains high for a critical period such that X and W can remain unstable arbitrarily long. The voltages at X and W

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as a function of time are described by the following set of differential equations when the drive transistor is non-conducting:

$$\frac{dV_W}{dt} = -\frac{I_W}{C_W} - \frac{\rho_X \cdot I_X}{C_X}$$

$$\frac{dV_X}{dt} = -\frac{I_X}{C_X} - \frac{\rho_W \cdot I_W}{C_W} \tag{1}$$

where V_X and V_W are the voltages at points X and W respectively, I_X and I_W are currents, C_X and C_W capacitances and ρ_X and ρ_W are coupling parameters with numerical values between 0 and 1. At equilibrium we have $I_W = I_X = 0$. The state of the circuit is completely specified by V_X and V_W (the source- and drain-voltages V_y and V_z are assumed to be constant) when the drive-transistor is non-conducting, so in this case we have a 2-dimensional phase space spanned by V_X and V_W. In this phase space there are three equilibrium points. Two of them correspond to the stable states with V_X high and V_W low or the other way round, whereas the third equilibrium point is unstable. In the vicinity of this third point the relation between currents and voltages is quadratic, because the conducting transistors are there in a so called saturated state:

$$I_W = \frac{1}{2}B_p(V_X - V_y - V_{tp})^2 + \frac{1}{2}B_n(V_X - V_z - V_{tn})^2$$

$$I_X = \frac{1}{2}B_p(V_W - V_y - V_{tp})^2 + \frac{1}{2}B_n(V_W - V_z - V_{tn})^2 \tag{2}$$

where V_{tp} and V_{tn} denote threshold voltages of the p- and n-transistors respectively, V_y and V_z are the source and ground voltage respectively and B_p and B_n are (transistor dependent) constants. In general we have $B_p < 0$ and $B_n > 0$. The capacitances C_W and C_X and the coupling parameters ρ_W and ρ_X are related by two other capacitances C_1 and C_2 according to

$$C_W = C_1 + \rho_W C_2$$

$$C_X = C_2 + \rho_X C_1 \tag{3}$$

but the background of all these relations will be irrelevant in the sequel. Next we want to calculate the unstable equilibrium point, given some specific numbers. Suppose $V_y = 5$ and $V_z = 0$(volts), $V_{tp} = -V_{tn} = -1$ and $B_p = -\frac{1}{4}B_n$. Equilibrium is defined by $\dot{V}_W = \dot{V}_X = 0$, where "$\cdot$" denotes differentiation with respect to time. Since $\rho_W < 1$ and $\rho_X < 1$ and $C_W > 0$ and $C_X > 0$ it follows from equations 1 that at equilibrium we must have $I_W = I_X = 0$, as remarked before. To find the unstable equilibrium point we need equations 2. This yields

$$I_W = 0$$
$$I_X = 0$$
$$\equiv \quad \{2\}$$

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$$\frac{1}{2}B_p(V_X - 4)^2 + \frac{1}{2}B_n(V_X - 1)^2 = 0$$

$$\frac{1}{2}B_p(V_W - 4)^2 + \frac{1}{2}B_n(V_W - 1)^2 = 0$$

$$\equiv \quad \{\text{calculus}\}$$

$$\frac{1}{2}(B_p + B_n)V_X^2 - (4B_p + B_n)V_X + 8B_p + \frac{1}{2}B_n = 0$$

$$\frac{1}{2}(B_p + B_n)V_W^2 - (4B_p + B_n)V_W + 8B_p + \frac{1}{2}B_n = 0$$

$$\equiv \quad \{B_p = -\tfrac{1}{4}B_n\}$$

$$\frac{3}{8}B_nV_X^2 - \frac{3}{2}B_n = 0$$

$$\frac{3}{8}B_nV_W^2 - \frac{3}{2}B_n = 0$$

$$\equiv \quad \{\text{calculus}\}$$

$$V_X^2 = 4 \quad \text{and} \quad V_W^2 = 4$$

$$\Rightarrow \quad \{\text{conducting transistors in saturated state}\}$$

$$V_X = V_W = 2$$

In order to linearise differential equations 1 in the neighbourhood of this unstable equilibrium point, we first rewrite the currents I_W and I_X:

$$I_W = \frac{3}{8}B_n[4(V_X - 2) + (V_X - 2)^2]$$

$$I_X = \frac{3}{8}B_n[4(V_W - 2) + (V_W - 2)^2] \tag{4}$$

So neglecting the quadratic terms in the neighbourhood of $V_X = V_W = 2$ gives:

$$I_W \approx \frac{3}{2}B_n(V_X - 2)$$

$$I_X \approx \frac{3}{2}B_n(V_W - 2) \tag{5}$$

Using this approximation we may write equations 1 in matrix form as:

$$\begin{pmatrix} (V_W - 2) \\ (V_X - 2) \end{pmatrix} = -\frac{3}{2}B_n \begin{pmatrix} \rho_X/C_X & 1/C_W \\ 1/C_X & \rho_W/C_W \end{pmatrix} \begin{pmatrix} (V_W - 2) \\ (V_X - 2) \end{pmatrix} \tag{6}$$

This may be written in shorthand form as $\underline{\dot{x}} = M\underline{x}$, where $\underline{x}$ stands for the vector $\begin{pmatrix} (V_W - 2) \\ (V_X - 2) \end{pmatrix}$ and M for the matrix given above. The general solution of this equation is easily written down in terms of the eigenvalues λ^- and λ^+ of M and their corresponding eigenvectors $\underline{e}^-$ and $\underline{e}^+$ respectively:

$$\underline{x}(t) = x^-\underline{e}^- e^{\lambda^- t} + x^+\underline{e}^+ e^{\lambda^+ t} \tag{7}$$

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if $\underline{x}(0) = x^-\underline{e}^- + x^+\underline{e}^+$. The eigenvalues are given by

$$\lambda^- = -\frac{3}{2}B_n \cdot \left[\frac{-b + \sqrt{b^2 - 4c}}{2}\right]$$

$$\lambda^+ = -\frac{3}{2}B_n \cdot \left[\frac{-b - \sqrt{b^2 - 4c}}{2}\right] \tag{8}$$

where

$$b = -\left(\frac{\rho_X}{C_X} + \frac{\rho_W}{C_W}\right)$$

and

$$c = \frac{1}{C_X C_W} \cdot (\rho_X \rho_W - 1)$$

Since $C_X, C_W, B_n > 0$ and $0 < \rho_X, \rho_W < 1$ we have $\lambda^- < 0$ and $\lambda^+ > 0$. If we write $\underline{e}^- = \begin{pmatrix} e_1^- \\ e_2^- \end{pmatrix}$ and $\underline{e}^+ = \begin{pmatrix} e_1^+ \\ e_2^+ \end{pmatrix}$, then the components are related by:

$$e_2^- = -C_W \cdot \left(\frac{2\lambda^-}{3B_n} + \frac{\rho_X}{C_X}\right) \cdot e_1^-$$

$$e_2^+ = -C_W \cdot \left(\frac{2\lambda^+}{3B_n} + \frac{\rho_X}{C_X}\right) \cdot e_1^+ \tag{9}$$

We may choose $\underline{e}^-$ to lie in the first quadrant and $\underline{e}^+$ in the fourth. If we do so then for all values of $\underline{x}(0)$ within the operational range of the circuit x^- must be chosen negative. If we choose $x^+ = \epsilon$ ($\epsilon > 0$) then in $V_W - V_X$-space the phase point first moves slowly in the direction of the equilibrium point $(V_W, V_X) = (2, 2)$ and then in the direction of the new stable state $(V_W, V_X) = (5, 0)$ (provided ϵ is small enough), whereas if we choose $x^+ = -\epsilon$ it moves after passing the equilibrium point in the direction of the initial stable state $(V_W, V_X) = (0, 5)$. The smaller ϵ is chosen, the longer the phase point stays in the vicinity of the equilibrium point. If we choose $x^+ = 0$ then the phase point approaches the equilibrium point asymptotically. The linearised differential equation can only describe the phase point's trajectory in the vicinity of the equilibrium point. The important property of the asymptotic approach of the equilibrium point (which causes the metastable behaviour) remains valid for the nonlinear equations 1, however. Since apart from the case $x^+ = 0$ all trajectories eventually leave the neighbourhood of the unstable equilibrium point, this point is called a metastable equilibrium point. In the next sections we will see how it can be eliminated from phase space.

3 Changing some constants

Looking at equation 7 we see that the origin $(0, 0)$ is always an equilibrium point, no matter what the eigenvalues are. If the initial position of the phase point is close enough

to the origin, it may take an arbitrarily long time to leave the neighbourhood of the origin (if ever). Our first objective therefore is to exclude any behaviour as described by equation 7. To this end we must eliminate the possibility of linearisation of equations 1. Such a linearisation is always possible when at equilibrium the two terms depending on B_p and B_n in the expressions for I_W and I_X (see equations 2) cancel each other but are non-zero themselves. If they are both zero in the equilibrium point then the relation between current and voltage becomes purely quadratic in its neighbourhood and can no longer be linearised. This can easily be established by changing the constants V_y, V_z, V_{tp} and V_{tn} in such a way that $V_y + V_{tp} = V_z + V_{tn} = A$, where A is a new constant. Equations 2 now read:

$$I_W = \frac{1}{2}(B_p + B_n)(V_X - A)^2$$

$$I_X = \frac{1}{2}(B_p + B_n)(V_W - A)^2 \tag{10}$$

If we further suppose (for simplicity) that $C_X = C_W = C$ ($C > 0$) and $\rho_W = \rho_X = \rho$ ($0 < \rho < 1$) and if we rename $\frac{1}{2}(B_p + B_n) = B$ ($B > 0$) and $V_W - A = w$ and $V_X - A = x$, then equations 1 may be rewritten as

$$\frac{dw}{dt} = -\frac{B}{C}(x^2 + \rho w^2)$$

$$\frac{dx}{dt} = -\frac{B}{C}(w^2 + \rho x^2) \tag{11}$$

Dividing one equation by the other we find the differential equation that describes the majority of the possible trajectories in $w - x$-space:

$$\frac{dw}{dx} = \frac{x^2 + \rho w^2}{w^2 + \rho x^2} \tag{12}$$

This equation is not defined in the point $(w, x) = (0, 0)$ which is an (unstable) equilibrium point of (11) and therefore also a possible trajectory. The half-line $x = w$ for $w > 0$ is another possible trajectory. A phase point on this trajectory moves towards the origin, but never reaches it, since the time T needed to reach the origin starting from a point $(w, x) = (w_0, w_0)$ with $w_0 > 0$ is given by:

$$T = \int_{w_0}^{0} \frac{dw}{\dot{w}} = \frac{C}{B(1 + \rho)} \int_{0}^{w_0} \frac{dw}{w^2} = \infty \tag{13}$$

A similar argument applies to the half-line $x = w$ for $w < 0$: a phase point on this trajectory moves away from the origin, but the time needed to leave an infinitesimal neighbourhood of the origin is again infinite. A detailed analysis shows that the other trajectories run all from the first quadrant to the third on either one or the other side of the line $x = w$, bending around the origin in either the second or the fourth quadrant. Does a phase point moving along one of these other trajectories always pass the origin in a bounded

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time, i.e. is the time that the phase point's projection on the w-axis needs to travel from say $+a$ to $-a$ $(0 < a < \infty)$ bounded? The answer turns out to be no: for trajectories running arbitrarily close to the line $x = w$ the time needed to pass the origin may become arbitrarily large. This is because the right-hand sides of equations 11 satisfy the so called *Lipschitz-condition*. This is best explained by writing (11) in vector form:

$$\begin{pmatrix} \dot{w} \\ \dot{x} \end{pmatrix} = -\frac{B}{C} \begin{pmatrix} x^2 + \rho w^2 \\ w^2 + \rho x^2 \end{pmatrix} = \{\text{definition } \underline{f}\} \underline{f}(t, w, x) \tag{14}$$

The components of $\underline{f}$ are continuous functions of t, w and x and partially differentiable with respect to w and x, so $\underline{f}$ is also (locally) Lipschitz-continuous in $\begin{pmatrix} w \\ x \end{pmatrix}$, i.e. for all t, $\begin{pmatrix} w \\ x \end{pmatrix}$ and $\begin{pmatrix} \overline{w} \\ \overline{x} \end{pmatrix}$ there is a constant $L(w, x)$ such that

$$|\underline{f}(t, w, x) - \underline{f}(t, \overline{w}, \overline{x})| \leq L(w, x) \cdot \left| \begin{pmatrix} w \\ x \end{pmatrix} - \begin{pmatrix} \overline{w} \\ \overline{x} \end{pmatrix} \right| \tag{15}$$

where we have chosen as vector norm:

$$\left| \begin{pmatrix} a \\ b \end{pmatrix} \right| = |a| \ \mathbf{max} \ |b|$$

Since $\underline{f}$ is continuous in t and Lipschitz-continuous in $\begin{pmatrix} w \\ x \end{pmatrix}$ one of the main theorems in the theory of ordinary differential equations tells us that for each initial position $(w(0), x(0))$ of a phase point it's present position $(w(t), x(t))$ is uniquely determined and depends continuously on the initial position, i.e. for each t and $\delta > 0$ there is an ϵ such that $\left| \begin{pmatrix} w(t) - \overline{w}(t) \\ x(t) - \overline{x}(t) \end{pmatrix} \right| < \delta$ for all $\begin{pmatrix} \overline{w}(0) \\ \overline{x}(0) \end{pmatrix}$ with $\left| \begin{pmatrix} w(0) - \overline{w}(0) \\ x(0) - \overline{x}(0) \end{pmatrix} \right| < \epsilon$. So the closer a phase point's initial position is to the line $x = w$ (in the first quadrant), the longer it will take to pass the origin, because on that line the phase point would never reach the origin but only approach it asymptotically. So the origin still is a metastable point in spite of the modified relation between current and voltage. In the next section we describe a further modification of this relation.

4   Changing the technology

We now consider a not yet invented technology in which the relation between current and voltage of a transistor in it's "saturated state" is described by (maintaining the analogy with the previous discussion as much as possible):

$$\begin{aligned} I_W &= B|x|^\alpha \\ I_X &= B|w|^\alpha \end{aligned} \tag{16}$$

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where $\alpha > 0$. For $\alpha = 2$ we retain the previous case. The equations of motion now read:

$$\frac{dw}{dt} = -\frac{B}{C}(|x|^\alpha + \rho|w|^\alpha)$$

$$\frac{dx}{dt} = -\frac{B}{C}(|w|^\alpha + \rho|x|^\alpha) \tag{17}$$

To get rid of the minus-sign we introduce new variables $x := -x$ and $y := -w$. We also abbreviate the right-hand sides by introducing the functions p and q:

$$\dot{x} = \frac{B}{C}(|y|^\alpha + \rho|x|^\alpha) = p(|x|, |y|)$$

$$\dot{y} = \frac{B}{C}(|x|^\alpha + \rho|y|^\alpha) = q(|x|, |y|) \tag{18}$$

A phase point on the line $y = x$ in the third quadrant now moves towards the origin along this line, whereas in the first quadrant it moves away from it. A simple calculation shows that for $\alpha \geq 1$ the origin cannot be reached in a finite time, whereas for $0 < \alpha < 1$ it can. In the former case p and q are Lipschitz-continuous everywhere and the time needed to pass the origin along a trajectory close to the line $y = x$ is again unbounded, but in the latter case p and q are Lipschitz-continuous everywhere except in the origin. If now the phase point reaches the origin along the line $y = x$, many things can happen: it can stay in the origin (which still is an equilibrium point), it may continue to move along the line $y = x$ in the first quadrant or it may wait an arbitrary time in the origin before continuing its journey. How do we determine the time needed to pass the origin close to the line $y = x$? Is in fact that line the only trajectory that intersects the origin? We will later prove that it is and that all the other trajectories run on either one or the other side of this line from the third quadrant to the first, bending around the origin in either the second or the fourth quadrant. We conjecture that the closer a phase point's trajectory runs to the line $y = x$, the closer it's time needed to pass the origin between point P and point Q approximates the time a phase point needs to move along the line $y = x$ from the projection of P to the projection of Q on that line, provided that it doesn't stop or wait a while in the origin. In order to prove this conjecture we may without loss of generality take $P = (a, -a)$, where $0 < a < 1$. For Q we take the intersection of the line $y = -x + 2$ with the trajectory through P (there can be only one such trajectory on account of the Lipschitz-continuity outside the origin). If we put $Q = (b, y(b))$ then we have $b > 1$ and $0 < y(b) < 1$, which follows from the proof that will be given later on (see also fig.2). We could also have taken $P = (x(-b), -b)$ and $Q = (a, -a)$, but that would basically give the same proof, only with the roles of x and y interchanged. The case $P = (-a, a)$ (or $Q = (-a, a)$) also goes similarly. The points $P = (a, -a)$ and $Q = (b, y(b))$ have the property that their projection on the line $y = x$ is given by $(0,0)$ and $(1,1)$ respectively. If a phase point moves from $(0,0)$ to $(1,1)$ along the line $y = x$ without stopping in the origin, it's coordinates $x(t)$ and $y(t)$ are invertible functions of time, i.e. $t(x)$ and $t(y)$ are well defined and if $t(0) = 0$ then $x > 0$ if $t(x) > 0$ and $x < 0$ if $t(x) < 0$ (in our example we also have $t(x) = t(y)$ for $x = y$).

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In that case (for $0 < \alpha < 1$) the time needed to move from $(0,0)$ to $(1,1)$ is given by:

$$T(0) = \int_{t(0)}^{t(1)} dt = \int_0^1 \frac{dx}{\dot{x}} = \int_0^1 \frac{dx}{p(x,x)} = \int_0^1 \frac{dy}{q(y,y)}$$

By a similar argument the time needed to move from P to Q is given by:

$$T(a) = \int_a^b \frac{dx}{p(x,|y(x)|)} = \int_{-a}^{y(b)} \frac{dy}{q(x(y),|y|)}$$

Our conjecture can now be formulated as:

$$\lim_{a \downarrow 0} T(a) = T(0) \tag{19}$$

First we calculate an underbound for $T(a)$:

$$T(a)$$
$$= \quad \{ \text{ definition } T(a)\}$$
$$\int_a^b \frac{dx}{p(x,|y(x)|)}$$
$$\geq \quad \{ b > 1\}$$
$$\int_a^1 \frac{dx}{p(x,|y(x)|)}$$
$$\geq \quad \{ |y(x)| < x, \text{ see proof later on } \}$$
$$\int_a^1 \frac{dx}{p(x,x)}$$
$$= \quad \{ \text{ definition } T(0) \}$$
$$T(0) - \int_0^a \frac{dx}{p(x,x)}$$

$T(0)$ and the last integral do not exist for $\alpha \geq 1$: if $\alpha \geq 1$ we can infer from the last inequality that $T(a) \to \infty$ if $a \downarrow 0$.

Next we calculate an upperbound for $T(a)$ (for $0 < \alpha < 1$):

$$T(a)$$
$$= \quad \{ \text{ definition } T(a)\}$$
$$\int_{-a}^{y(b)} \frac{dy}{q(x(y),|y|)}$$
$$= \quad \{ \text{ calculus}\}$$
$$\int_{-a}^0 \frac{dy}{q(x(y),-y)} + \int_0^{y(b)} \frac{dy}{q(x(y),y)}$$
$$\leq \quad \{ \text{ first term: } x(y) \geq a \text{ and } \eta := -y; \text{ second term: } x(y) > y \text{ and } y(b) < 1 \}$$

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$$\int_0^a \frac{d\eta}{q(a,\eta)} + \int_0^1 \frac{dy}{q(y,y)}$$

$\leq \quad \{\ a \geq \eta,\ q(y,y) = p(y,y) \text{ and definition } T(0)\}$

$$T(0) + \int_0^a \frac{d\eta}{q(\eta,\eta)}$$

$= \quad \{\ q(\eta,\eta) = p(\eta,\eta)\ \}$

$$T(0) + \int_0^a \frac{d\eta}{p(\eta,\eta)}$$

Combining upper- and lowerbound yields:

$$|T(a) - T(0)| \leq \int_0^a \frac{dx}{p(x,x)}$$

$\Rightarrow \quad \{\text{ integral exists for } 0 < \alpha < 1\ \}$

$$\lim_{a \downarrow 0} T(a) = T(0)$$

which concludes our proof.

We still have to prove that there are no other trajectories through the origin than the line $y = x$. We may write the functions p and q as

$$p(|x|,|y|) = \rho f(|x|) + f(|y|)$$
$$q(|x|,|y|) = f(|x|) + \rho f(|y|) \tag{20}$$

where $f : [0,\infty) \to [0,\infty)$ is monotonically increasing and locally Lipschitz-continuous on $(0,\infty)$. Using f, all trajectories except the origin are determined by

$$(\rho f(|x|) + f(|y|))\frac{dy}{dx} = f(|x|) + \rho f(|y|) \tag{21}$$

We are interested in the behaviour of $\frac{dy}{dx}$ on the line $y = x - 2a$. For $x = a$ one can easily verify that $\frac{dy}{dx} = 1$, whereas for $x > a$ we claim: $\frac{dy}{dx} > 1$. Introducing the abbreviations

$$L = \rho f(x) + f(|x - 2a|)$$
$$R = f(x) + \rho f(|x - 2a|)$$

we can write our claim as $L < R$ for $x > a$. We prove this first for $a < x < 2a$:

$L < R$

$\equiv \quad \{\text{ definition } L \text{ and } R\ \}$

$\rho f(x) + f(2a - x) < f(x) + \rho f(2a - x)$

$\equiv \quad \{\text{ calculus }\}$

$(\rho - 1)f(x) < (\rho - 1)f(2a - x)$

$\equiv \quad \{\ 0 < \rho < 1\}$

$f(2a - x) < f(x)$

$\equiv \quad \{\ f \text{ monotonically increasing}\}$

$true$

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For $x \geq 2a$ we have:

$$L < R$$
$\equiv$ { definition L and R }
$$\rho f(x) + f(x - 2a) < f(x) + \rho f(x - 2a)$$
$\equiv$ { calculus }
$$(\rho - 1)f(x) < (\rho - 1)f(x - 2a)$$
$\equiv$ { $0 < \rho < 1$ }
$$f(x - 2a) < f(x)$$
$\equiv$ { f monotonically increasing }
$$true$$

Similarly for $x < a$ one can prove $0 < \frac{dy}{dx} < 1$. Since the argument is valid for any value of $a > 0$, it follows that the trajectory through $(a, -a)$ must lie entirely between the lines $y = x$ and $y = x - 2a$; the trajectory cannot intersect the line $y = x$ outside the origin since f is locally Lipschitz-continuous on $(0, \infty)$ and it can also not intersect the origin on account of the behaviour of $\frac{dy}{dx}$. Similarly, the trajectory through $(-a, a)$ lies entirely between the lines $y = x + 2a$ and $y = x$ (see fig.2). For the trajectory through $(a, -a)$ we observe that $|y(x)| < x$ for $x > a$. We have chosen $a < 1$ to ensure $y(b) > 0$: in that case the trajectory intersects the line $y = -x + 2$ in a point $(b, y(b))$ not only with $b > 1$ and $y(b) < 1$ (because $y(x) < x$), but also with $y(b) > 0$ because the lines $y = -x + 2$ and $y = x - 2a$ intersect in $(a + 1, -a + 1)$, $-a + 1 > 0$ for $a < 1$ and on the trajectory $y(x) \geq x - 2a$ holds. We could also have chosen a different intersection point Q with projection (c, c) on $y = x$ for some $c > 0$ by scaling a and b correspondingly. It wouldn't change the conclusion that the phase point always passes the origin in a finite time (for $\alpha < 1$) between P and Q which approaches the time to move from $(0,0)$ to (c,c) if P approaches the origin, provided that the phase point on the line $y = x$ doesn't wait in the origin.

Theoretically the origin is still an equilibrium point of the equations of motion. If we impose the well-posedness criterion however, which implies that the phase point's coordinates $x(t)$ and $y(t)$ shall vary continuously with the initial values $x(0)$ and $y(0)$, waiting in the origin is forbidden because $\lim_{a \downarrow 0} T(a) = T(0)$. The origin is therefore no longer a metastable point, but only a point where $\dot{x} = \dot{y} = 0$ for a single moment in time. Nevertheless, if we look at fig.2 we see that the trajectories run parallel to the line $y = x$ asymptotically, so they cannot diverge to different stable points in phase space if they pass the origin nearby. In the next section we will see how this can be changed as well.

5 Changing a parameter

Looking again at the derivation of $L < R$ for $x > a$, we see that the hint $\rho < 1$ plays a crucial role; had it been $\rho > 1$ then we would have found $L > R$ or (equivalently) $\frac{dy}{dx} < 1$
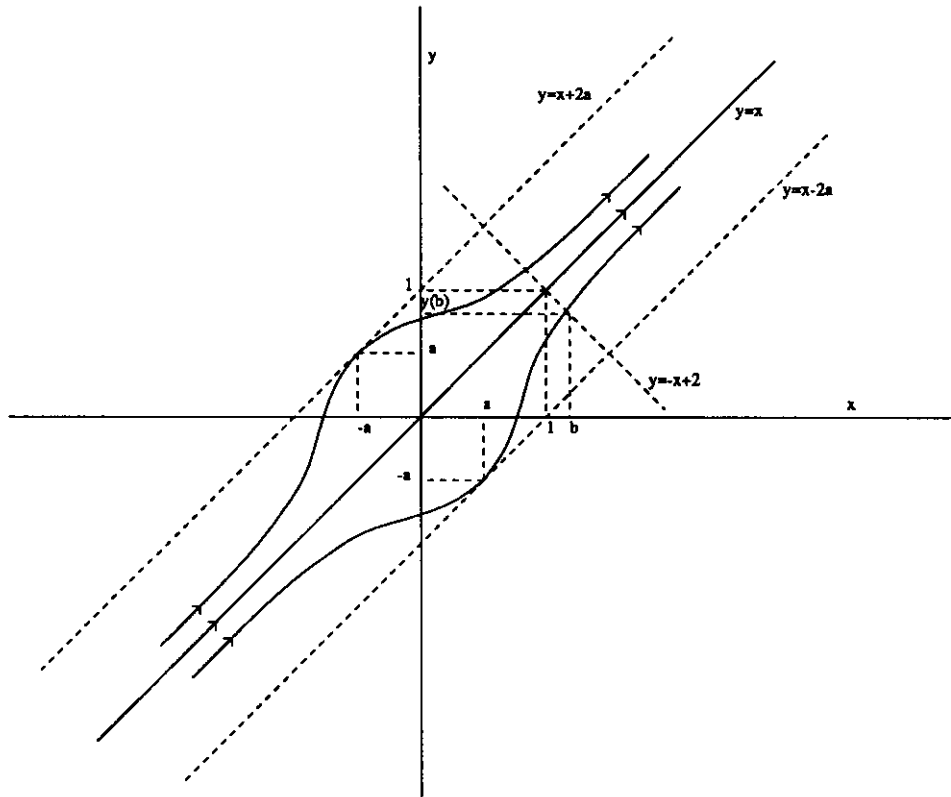
Figure 2: Phase portrait for $0 < \rho < 1$.

for $x > a$. Since $L > 0$ and $R > 0$ we also have $0 < \frac{dy}{dx}$. For $x = a$ we would have $\frac{dy}{dx} = 1$ as before and for $x < a$ we would have found $\frac{dy}{dx} > 1$. Reflection of this trajectory with respect to the line $y = x$ would give a new trajectory as before, leading to a phase portrait as sketched in fig.3. As one can see in that figure, now the trajectories diverge from the line $y = x$. So let us suppose $\rho > 1$. It can be proven again (for $0 < \alpha < 1$) that $\lim_{a \downarrow 0} T(a) = T(0)$, so imposing the well-posedness criterion leads to elimination of the metastable point in the origin as before. Can we now say that metastable behaviour has been eliminated as well? Unfortunately not. The well-posedness criterion implies that trajectories depend continuously on initial conditions, so for $a \downarrow 0$ the trajectory through $(a, -a)$ (or through $(-a, a)$) will run almost parallel to the line $y = x$. It may therefore take an arbitrary long time for a phase point moving along such a trajectory to bend away from the line $y = x$ and reach a stable point, so metastable behaviour is still possible. Note that the equations of motion are only supposed to hold in the neighbourhood of the origin, but extending the locally valid phase portrait of fig.3 to the entire phase space cannot prevent metastable behaviour unless a new stable point is introduced (which is undesirable as it leads to unreliable switching of the circuit) or if trajectories are allowed to have sharp corners or to intersect (which is forbidden). As mentioned in the introduction the formal proof that the well-posedness criterion makes metastable behaviour unavoidable can be
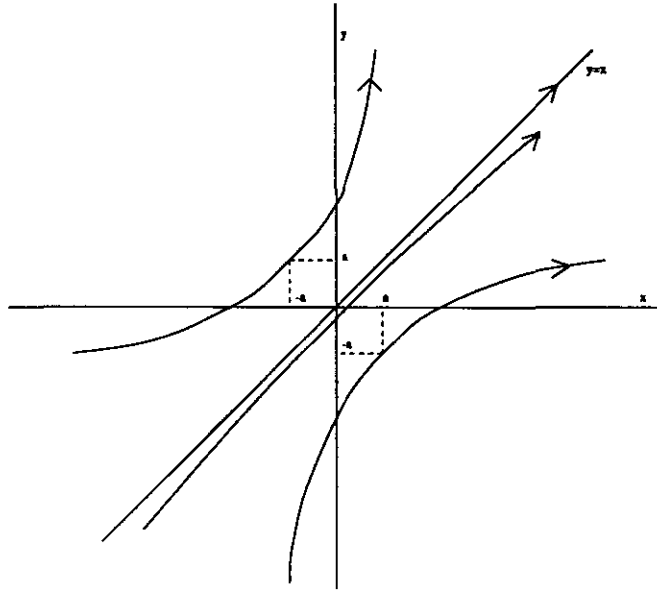
Figure 3: Phase portrait for $\rho > 1$.

found in [Hur75], [Mar81] or [KC87].

Metastability can therefore only be eliminated if the well-posedness criterion is somehow violated. An obvious violation is to introduce a branch point somewhere on the line $y = x$: if a phase point moving along this line reaches the branch point it can either turn right or left (see fig.4), moving to one stable point or the other. Metastability is

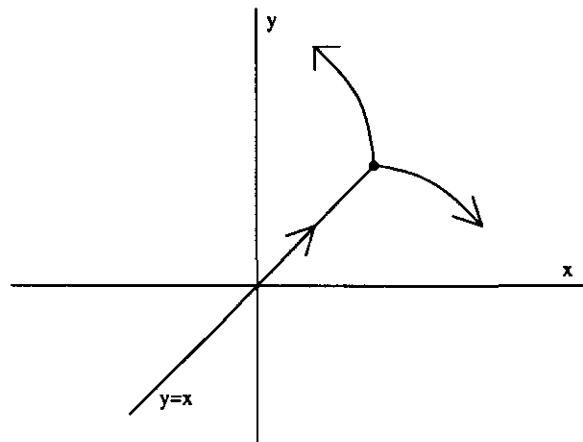Figure 4: A branch point on the line $y = x$.

eliminated if the branch point can be reached in a finite time (otherwise this point would be called a bifurcation point). Trajectories can now no longer depend continuously on initial conditions: at best we can have the trajectory through $(-a, a)$ running very closely to the line $y = x$ and the left branch and the trajectory through $(a, -a)$ running very

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closely to the line $y = x$ and the right branch for $a \downarrow 0$. In the next section we give an example of a (perhaps non-physical) system with such a branching trajectory and show how metastability is eliminated under the assumption of semi-continuity.

6 Particle on the hill

An example of a bistable system is a particle with mass m which can move from one hole to another by passing a hill in between. The holes are supposed to have some trapping device to prevent the particle's escape from a hole, unless some external force is applied. In the example of the mousetrap circuit we were only interested in the region of phase space where transistors were in their saturated state (which included the metastable point), here we are only interested in the particle's behaviour on the hill between the two holes, in particular near the top.

Suppose the hill is described by the function

$$y(x) = y_0 - |x_0 - x|^\alpha \tag{22}$$

where $y_0 = x_0^\alpha$, $x_0 > 0$ and $\alpha > 1$ (see fig.5). The particle's x- and y-coordinates are
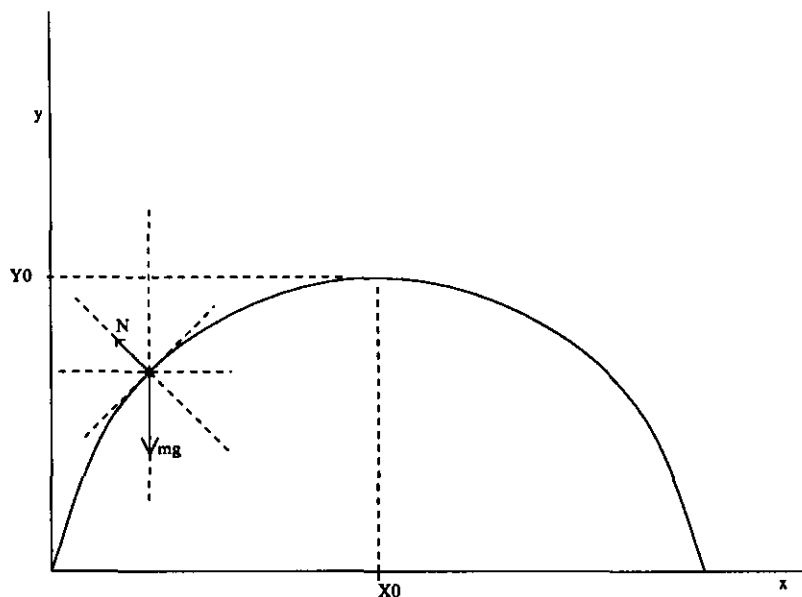
Figure 5: Particle on the hill.

functions of time that satisfy Newton's equations of motion: $m\ddot{x} = R_x$ and $m\ddot{y} = R_y$ (the dots denote differentiation with respect to time), where R_x and R_y are the x- and y-components of the total force $\vec{R}$ acting on the particle. $\vec{R}$ is the vector-sum of the gravitational force $m\vec{g}$ and the normal force $\vec{N}$:

$$\vec{R} = m\vec{g} + \vec{N} \tag{23}$$

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This yields for the components of $\vec{R}$: $R_x = N_x$ and $R_y = N_y - mg$. The components of $\vec{N}$ are related by:

$$\frac{N_y}{N_x} = -\frac{1}{y'(x)} \tag{24}$$

except in the top where $N_x = 0$. The prime denotes differentiation with respect to x. When $N_y < 0$ the normal force points inside the hill, which is actually impossible for a particle on a hill because in that case the gravitational force is not strong enough to keep the particle on the hill. For a particle moving along a cable (or curtain rail) with the same shape it is very well possible though. Here we do not bother about such details, since we are only interested in the equations of motion. We derive:

$$\ddot{y}$$
$$= \quad \{ \text{ definition} \}$$
$$\frac{d}{dt}(y(x(t)))$$
$$= \quad \{ \text{ calculus} \}$$
$$y'(x) \cdot \dot{x}$$
$$\Rightarrow \quad \{ \text{ calculus} \}$$
$$\ddot{y} = y''(x) \cdot (\dot{x})^2 + y'(x) \cdot \ddot{x}$$
$$\equiv \quad \{ m\ddot{y} = N_y - mg \}$$
$$my''(x) \cdot (\dot{x})^2 + y'(x) \cdot m\ddot{x} = N_y - mg$$
$$\Rightarrow \quad \{ \text{ define } p = m\dot{x} \text{ and } N_y = -\dot{p}/y'(x) \}$$
$$y''(x) \cdot y'(x) \cdot \frac{p^2}{m} + (y'(x))^2 \cdot \dot{p} = -\dot{p} - mgy'(x)$$
$$\equiv \quad \{ \text{ calculus} \}$$
$$\dot{p} = -[1 + (y'(x))^2]^{-1} \cdot \left(y''(x) \cdot \frac{p^2}{m} + mg \right) \cdot y'(x)$$

We represent the particle on the hill by a phase point $(x(t), p(t))$ whose trajectory is described by the following equations:

$$\dot{x} = \frac{p}{m}$$
$$\dot{p} = -[1 + (y'(x))^2]^{-1} \cdot \left(\frac{p^2}{m} \cdot y''(x) + mg \right) \cdot y'(x) \tag{25}$$

Using these equations one can prove that

$$\frac{p^2}{2m} \cdot [1 + (y'(x))^2] + mgy(x)$$

is a constant function of time (usually called the total energy). Suppose $x(0) = 0$. It can be easily verified -using conservation of total energy- that if $\frac{p^2(0)}{2m} \cdot [1 + (y'(0))^2] = mgy_0$

and $p > 0$ then at the top of the hill $p = 0$. The condition $p > 0$ is only to assure that the particle is moving from the origin to the top of the hill; for $p < 0$ we have a similar relation, but then for a particle moving backwards from the top to the origin. The time T needed to reach the top such that at the top $p = 0$ holds can be calculated as follows. For all x, $0 \leq x \leq x_0$, we have (using again conservation of energy):

$$\frac{p^2}{2m} \cdot [1 + (y'(x))^2] + mgy(x) = mgy_0$$

$$\equiv \quad \{ \text{calculus} \}$$

$$p^2 = \frac{2m}{1 + (y'(x))^2} \cdot mg(y_0 - y(x))$$

$$\Rightarrow \quad \{ p > 0 \}$$

$$p = m\sqrt{\frac{2g(y_0 - y(x))}{1 + (y'(x))^2}} = m\dot{x}$$

$$\Rightarrow \quad \{ \text{definition } T \text{ and calculus} \}$$

$$T = \int_0^{x_0} \frac{dx}{\dot{x}} = \int_0^{x_0} dx \sqrt{\frac{1 + (y'(x))^2}{2g(y_0 - y(x))}}$$

Substitution of (22) in this expression for T shows that for $\alpha \geq 2$ the top will never be reached (i.e. $T = \infty$), whereas for $1 < \alpha < 2$ it will be reached in a finite time. If we choose $p < 0$ in the derivation above, we find that T is also the time needed to move from the top backwards to the origin when initially $p = 0$ and since the hill is symmetric around $x = x_0$, T is also the time needed to move from $x = x_0$ to $x = 2x_0$ or vice versa for the same initial condition $p = 0$. For $1 < \alpha < 2$ we may therefore conclude that the phase point needs a time $2T$ to move from $x = 0$ to $x = 2x_0$ if its trajectory intersects the point $(x_0, 0)$, provided that the particle doesn't spend time waiting on top of the hill, since in that case $\dot{x}$ is not only zero at a single moment in time but zero during some consecutive time-interval so that the time-integral cannot be transformed into a space-integral such as appears in the expression for T.

For $\alpha \geq 2$ we have the same metastable behaviour as before, whereas for $1 < \alpha < 2$ something completely new happens. The point $(x_0, 0)$ in phase space still is an equilibrium point of the equations of motion (25) where the phase point can stay for an arbitrary time before moving on (due to violation of the Lipschitz-condition), but now it is also a branch point where an incoming trajectory representing a particle climbing the hill splits into a trajectory representing a particle rolling off the hill on the other side as where it came from and a trajectory representing a particle rolling backwards. The resulting phase portrait is shown in fig.6. Note that in this phase portrait we have actually assumed $1\frac{1}{2} < \alpha < 2$ (so that for the upper trajectory $\frac{dp}{dx} = 0$ in $x = x_0$), since otherwise R_x would be non-zero at the top of the hill ($\frac{dp}{dx} = \infty$ for $1 < \alpha < 1\frac{1}{2}$ and $0 < \frac{dp}{dx} < \infty$ for $\alpha = 1\frac{1}{2}$ in $x = x_0$ if $p(x_0) > 0$), which is unphysical.

In order to remove the equilibrium solution $(x_0, 0)$ we can now no longer impose the well-posedness criterion; at best we can have the upper trajectory approximating the incoming
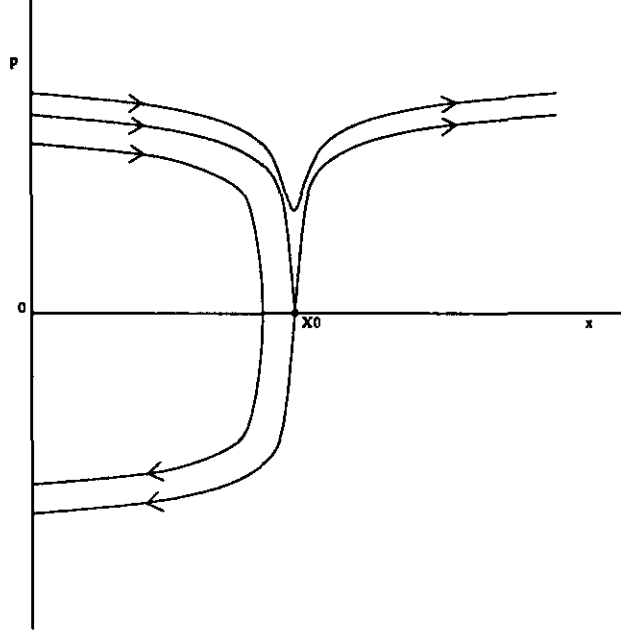
Figure 6: Phase portrait for $1\frac{1}{2} < \alpha < 2$.

trajectory and the outgoing upper branch and the lower trajectory approximating the incoming trajectory and the outgoing lower branch. These approximations can become arbitrarily close if we impose a new type of continuity condition, which we shall refer to as semi-continuity, for the reason given above. If we suppose for $0 \le c < x_0^\alpha$

$$\frac{p^2}{2m} \cdot [1 + (y'(x))^2] + mgy(x) = mg(y_0 \pm c) \tag{26}$$

then in case of the $+$-sign the particle needs a time $T^+(c)$ to reach the top, given by

$$T^+(c) = \int_0^{x_0} dx \sqrt{\frac{1 + (y'(x))^2}{2g(y_0 + c - y(x))}} \tag{27}$$

and in case of the $-$-sign the particle needs a time $T^-(c)$ to reach $x_0 - c^{1/\alpha}$, given by

$$T^-(c) = \int_0^{x_0-c^{1/\alpha}} dx \sqrt{\frac{1 + (y'(x))^2}{2g(y_0 - c - y(x))}} \tag{28}$$

(after this time the particle moves back to the origin). Note that $T^+(0) = T^-(0) = T$. If we restrict ourselves to solutions $(x(t), p(t))$ of (25) with $x(0) = 0$, the semi-continuity

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condition may be formulated for every $t \geq 0$ as follows:

$$(\forall \epsilon : \epsilon > 0 : \quad (\exists \delta : \delta > 0 : \quad (\forall (\overline{x}(0), \overline{p}(0)) : \quad \overline{x}(0) = 0 \wedge 0 < \overline{p}(0) - p(0) < \delta :$$
$$|\overline{x}(t) - x(t)| < \epsilon$$
$$)$$
$$\vee$$
$$(\forall (\overline{x}(0), \overline{p}(0)) : \quad \overline{x}(0) = 0 \wedge 0 < p(0) - \overline{p}(0) < \delta : \quad (29)$$
$$|\overline{x}(t) - x(t)| < \epsilon$$
$$)$$
$$)$$
$$)$$

We have deliberately not chosen the most general formulation, but one that is sufficient for our purposes. For solutions $(x(t), p(t))$ with $p(t) = 0$ if $x(t) = x_0$ at most one of the disjuncts can be true, whereas for all other solutions both disjuncts are true. If none of the disjuncts is true then the particle is waiting on top of the hill. This follows from the fact that $\lim_{c \downarrow 0} T^+(c) = T^+(0)$ and $\lim_{c \downarrow 0} T^-(c) = T^-(0)$ which we shall prove below. So if we impose this semi-continuity condition on the set of solutions of (25) (and assuming $x(0) = 0$ for convenience) all solutions where the particle is waiting on top of the hill are excluded, thereby completely eliminating metastable behaviour (still assuming $1 < \alpha < 2$, of course). In order to prove our claim about $T^+(c)$ and $T^-(c)$, we need the following lemma:

$$\frac{1}{\sqrt{1+u}} = 1 + O(u)$$

for $u \geq -\beta$ with $0 < \beta < 1$. One may prove this by considering the function $h(u)$, given by

$$h(u) = \frac{(1+u)^{-\frac{1}{2}} - 1}{u}$$

If we define $h(0) = -\frac{1}{2}$, then h is continuous on $[-\beta, \infty)$. Since $|h(-\beta)|$ is bounded and $\lim_{u \to \infty} h(u) = 0$, there must exist a constant $M(\beta)$ such that

$$(\forall u : -\beta \leq u : |h(u)| \leq M(\beta))$$

which proves the lemma. If we define the functions $t^+(c)$ and $t^-(c)$ for $0 \leq c < x_0^\alpha$ by

$$t^+(c) = \int_0^{x_0} \frac{dx}{\sqrt{(x_0 - x)^\alpha + c}}$$

$$t^-(c) = \int_0^{x_0 - c^{1/\alpha}} \frac{dx}{\sqrt{(x_0 - x)^\alpha - c}} \quad (30)$$

then the following inequalities hold:

$$|T^\pm(c) - T^\pm(0)| \leq \sqrt{\frac{1 + \alpha^2 x_0^{2\alpha - 2}}{2g}} |t^\pm(c) - t^\pm(0)| \quad (31)$$

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Because

$$t^+(0) = t^-(0) = \int_0^{x_0} \frac{dx}{\sqrt{(x_0 - x)^\alpha}}$$

we can derive for $c < x_0^\alpha$:

$t^+(c)$

$=$ { definition}

$$\int_0^{x_0} dx \sqrt{\frac{1}{c + (x_0 - x)^\alpha}}$$

$=$ $\{ y = x_0 - x \}$

$$\int_0^{x_0} dy \sqrt{\frac{1}{c + y^\alpha}}$$

$=$ $\{ c = a^\alpha \}$

$$\int_0^{x_0} \frac{dy}{\sqrt{a^\alpha + y^\alpha}}$$

$=$ $\{ y = az \}$

$$a^{1-\frac{1}{2}\alpha} \int_0^{x_0/a} \frac{dz}{\sqrt{1 + z^\alpha}}$$

$=$ { calculus}

$$a^{1-\frac{1}{2}\alpha} \cdot \left(\int_0^1 \frac{dz}{\sqrt{1 + z^\alpha}} + \int_1^{x_0/a} dz \frac{z^{-\alpha/2}}{\sqrt{1 + z^{-\alpha}}} \right)$$

$=$ { lemma}

$$a^{1-\frac{1}{2}\alpha} \cdot \left(\int_0^1 \frac{dz}{\sqrt{1 + z^\alpha}} + \int_1^{x_0/a} dz z^{-\alpha/2} \cdot (1 + O(z^{-\alpha})) \right)$$

$=$ { calculus}

$$t^+(0) + O(a^{1-\frac{1}{2}\alpha})$$

and for $c < \left(\frac{x_0}{2} \right)^\alpha$ we can derive

$t^-(c)$

$=$ { definition}

$$\int_0^{x_0 - c^{1/\alpha}} dx \frac{1}{\sqrt{(x_0 - x)^\alpha - c}}$$

$=$ $\{ c = a^\alpha \}$

$$\int_0^{x_0 - a} \frac{dx}{\sqrt{(x_0 - x)^\alpha - a^\alpha}}$$

$=$ $\{ y = x_0 - x \}$

$$\int_a^{x_0} \frac{dy}{\sqrt{y^\alpha - a^\alpha}}$$

$$= \quad \{ y = az \}$$
$$a^{1-\alpha/2} \int_1^{x_0/a} \frac{dz}{\sqrt{z^\alpha - 1}}$$
$$= \quad \{ \text{calculus} \}$$
$$a^{1-\alpha/2} \cdot \left(\int_1^2 \frac{dz}{\sqrt{z^\alpha - 1}} + \int_2^{x_0/a} dz \frac{z^{-\alpha/2}}{\sqrt{1 - z^{-\alpha}}} \right)$$
$$= \quad \{ \text{lemma} \}$$
$$a^{1-\alpha/2} \cdot \left(\int_1^2 \frac{dz}{\sqrt{z^\alpha - 1}} + \int_2^{x_0/a} dz z^{-\alpha/2} \cdot (1 + O(z^{-\alpha})) \right)$$
$$= \quad \{ \text{calculus} \}$$
$$t^-(0) + O(a^{1-\alpha/2})$$

We can now infer from the inequalities (31) and the definition $c = a^\alpha$ that

$$|T^\pm(c) - T^\pm(0)| = O(c^{\frac{1}{\alpha} - \frac{1}{2}}) \tag{32}$$

Hence, for $1 < \alpha < 2$:

$$\lim_{c \downarrow 0} T^\pm(c) = T^\pm(0) = T \tag{33}$$

which concludes the proof of the claim we made before. Note that it also holds for the unphysical range $1 < \alpha \le 1\frac{1}{2}$.

7 Is metastability avoidable?

In the previous section we have seen an example of a bistable system without metastable behaviour. The question is of course whether such a system can be physically realised. At first sight there seems to be nothing unphysical about a particle on a hill for $1\frac{1}{2} < \alpha < 2$. The violation of the well-posedness condition is a serious matter of course, but the semi-continuity condition preserves much of the old concept. In this context it is interesting to note a recent paper in the physics literature by Michail Zak [Zak92]. He demonstrates how violation of the Lipschitz condition (which in his case amounts to violation of the well-posedness condition) in systems that can exchange energy with their environment can give a new explanation for chaotic phenomena, leading to a new type of chaos which he calls terminal chaos. In this type of chaos equilibrium points can be approached in a finite time and also left following different branches of the same incoming trajectory, very much like the particle on the hill in the previous section.

To see whether the particle on the hill can be physically realised, one should take the microscopic structure of the particle and the hill into account. Both are composed of atoms and molecules which interact with each other through some potential function. If one still assumes Newton's equations of motion to be valid at this microscopic level, everything depends on the potential function. When the potential function has some standard form (like Lennard-Jones), it seems likely that the particle on the hill (for $1\frac{1}{2} < \alpha < 2$) cannot

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be realised, because it is hard to imagine how the Lipschitz-condition can be violated for smooth potentials that only become infinitely repulsive at some distance between molecules. Actually Newton's equations of motion are not valid at the microscopic level and only quantum mechanics can give a reliable description of the interaction between two atoms or molecules. For a macroscopic number of atoms or molecules the macroscopic behaviour can often very well be approximated by assuming the validity of classical mechanics at the microscopic level. Often is not always, however. For instance, if water is in a so called undercooled state, it can change into ice immediately after a very small disturbance in the water. At the microscopic level the water molecules form so called hydrogen bonds between hydrogen atoms in different water molecules. The question seems legitimate whether phase transitions like these still obey the well-posedness criterion, i.e. whether in this case a physical transition point exists between the state of undercooled water and the state of ice such that the system can spend an indefinite period of time in the transition point. No definite answer seems available to date, but traditionally the phenomenon of critical slowing down is associated with second order phase transitions (where thermodynamical quantities change continuously, but their derivatives not) and not with first order phase transitions (where thermodynamical quantities change discontinuously) like the one from water to ice. In this case the absence of a physical transition point would ultimately stem from the quantum mechanical nature of the formation of hydrogen bonds between water molecules and the formation of a crystal structure out of these bonds. If true, then Marino and others are wrong in supposing that the well-posedness criterion applies to all physical systems. Sometimes people make the more modest claim that it applies to all classical physical sytems, but it seems somewhat odd to consider water and ice as non-classical physical systems.

Since no definite answer seems available to date, we will now focus on systems that are truly quantum mechanical. Our motivation for doing so stems from the particle on the hill example of the previous section. In case $\alpha = 1$ we don't have a hill, but a roof formed by the line-segments $y = x$ for $0 \leq x \leq x_0$ and $y = 2x_0 - x$ for $x_0 \leq x \leq 2x_0$. The total force acting on the particle is now no longer defined at the top of the roof (i.e. for $x = x_0$), but we can define it as a random variable with two possible values, one being equal to the value of the force for $x < x_0$ and the other one equal to the value for $x > x_0$. If we do so then an incoming trajectory representing a particle reaching the top with zero velocity branches into a trajectory representing a particle moving to the left and a trajectory representing a particle moving to the right. Again, there is no metastability because the total force has always the same positive magnitude (but two different directions are possible). Rooves with such a sharp top are certainly not physically realisable on a macroscopic scale, but in quantum mechanics we face a new situation. We can define for each (fermion) particle a trajectory using a so called quantum potential. Adding this quantum potential to the classical potential and using Newton's equations of motion like in classical mechanics, we can calculate the trajectory. We can not observe the trajectory, however. We can calculate all trajectories corresponding to a set of initial conditions and the probability that these initial conditions are within a certain range, but we can only observe certain quantities that are averaged over all possible trajectories according to the probability distribution over

the set of initial conditions. There is an ongoing metaphysical debate about the status of quantum mechanics, for instance whether the trajectories mentioned above really exist or not, but here we only use them to make judgments about observable quantities. The nice thing about the quantum potential is that it facilitates the construction of roof-like potentials with a perfectly sharp top, as we shall demonstrate now.

We consider a particle with mass m and position $\vec{r}$ moving under the influence of a potential $V(\vec{r})$. With the particle is associated a wave function $\psi(\vec{r}, t)$ which determines both the possible trajectories of the particle and the probability distribution over the possible initial conditions. Given $\psi(\vec{r}, 0)$ we can calculate the wave function for all times t by solving the following partial differential equation, usually called the Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V\psi \tag{34}$$

where $\hbar$ is a constant of nature and $\vec{\nabla}^2$ is a differential operator given by $\vec{\nabla}^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, which may also be written symbolically as $\vec{\nabla}\cdot\vec{\nabla}$ where $\vec{\nabla}$ is the gradient operator. Writing

$$\psi = Re^{iS/\hbar}$$

where $R(\vec{r}, t)$ and $S(\vec{r}, t)$ are real functions and $R = |\psi|$, we can decompose the Schrödinger equation in a real and imaginary part. After some manipulations that involve multiplication of right- and left-hand sides of one equation with R and dividing left- and right-hand sides of the other equation by R (which is allowed for $R \neq 0$), we find:

$$\begin{aligned}\frac{\partial S}{\partial t} + \frac{(\vec{\nabla}S)^2}{2m} + V + Q &= 0 \\ \frac{\partial P}{\partial t} + \vec{\nabla}\cdot\frac{(P\vec{\nabla}S)}{m} &= 0\end{aligned} \tag{35}$$

where

$$Q = \frac{-\hbar^2}{2m}\cdot\frac{\vec{\nabla}^2 R}{R}$$

and

$$P = R^2$$

$Q(\vec{r}, t)$ is the quantum potential and $P(\vec{r}, t)$ is the probability density for finding the particle at position $\vec{r}$ at time t. The possible trajectories of the particle are found by interpreting $\vec{\nabla}S$ as the impulse of the particle, i.e. $m\dot{\vec{r}} = \vec{\nabla}S$, where $\vec{r}$ is now an implicit function of time and the dot denotes differentiation with respect to time. Integration of the impulse over time then gives the trajectory; the different integration constants that are still allowed correspond to the possible initial positions. Note that the initial impulse can no longer be varied independently, but is fixed by the initial position. This interpretation was first given by David Bohm in 1952. As said before, we will only use it to discuss observable phenomena like metastability. With this interpretation the second equation in (35) guarantees conservation of probability and the first equation becomes the Hamilton-Jacobi equation

for a total potential $V + Q$; it can be rewritten as Newton's equation of motion by taking the gradient of left- and right-hand sides and rewriting the first two terms as a total time derivative of $\vec{\nabla}S$:

$$m\ddot{\vec{r}} = -\vec{\nabla}(V + Q)$$

This shows that quantum mechanics may be approximated by classical mechanics whenever the quantum potential Q is negligible compared to the classical potential V. Although the initial impulse is fixed by the initial position, the initial wave function $\psi(\vec{r}, 0)$ may still be varied. This gives the freedom to change not only the initial impulse but the quantum potential as well.

To show a roof-like quantum potential we assume for simplicity that the wave function only depends on the x-coordinate of the particle. Now suppose $\psi(0) = 0$ at some point in time, and suppose further that

$$\text{for } x < 0 \quad : \quad \psi(x) = x + \frac{1}{6}ax^3 + \frac{1}{12}b_- x^4$$

$$\text{for } x > 0 \quad : \quad \psi(x) = x + \frac{1}{6}ax^3 + \frac{1}{12}b_+ x^4$$

then if $x \to 0$:

$$\frac{|\psi(x)|''}{|\psi(x)|} \to a$$

and

$$\text{for } x \downarrow 0 \quad : \quad \frac{d}{dx}\left[\frac{|\psi(x)|''}{|\psi(x)|}\right] \to b_+$$

$$\text{for } x \uparrow 0 \quad : \quad \frac{d}{dx}\left[\frac{|\psi(x)|''}{|\psi(x)|}\right] \to b_-$$

For a and b_- positive and b_+ negative the quantum potential has indeed the shape of a roof (the signs are just the opposite if one includes the constant factor in Q). A weak point may be that for this choice of ψ the fourth derivative doesn't exist in $x = 0$. Strictly speaking the existence of a fourth derivative (with respect to x) is not required for a solution of the Schrödinger equation, but perhaps such solutions are unphysical. Actually one should not look at the wave function for one moment in time as we did, but rather consider the evolution in time.

Let us consider in one dimension a so called square well potential, i.e. $V(x) = 0$ for $x < 0.718$ and $x > 0.782$ and in between $V(x) = -2(50\pi)^2$. For simplicity we take such units that $\hbar = 1$ and $m = 0.5$. Suppose the initial wave function is given by

$$\psi(x, o) = \exp[ik_0 x]\exp[-(x - x_0)^2/2\sigma_0^2]$$

where $k_0 = 50\pi$, $x_0 = 0.5$ and $\sigma_0 = 0.05$. This represents a particle incident on the square well from the left (i.e. from $x < 0.718$) with an average energy equal to half the well depth. Two things can happen: the particle crosses the well or it is reflected. A third possibility

would be that the particle is trapped inside the well, which would be a metastable state. Whether a particle is transmitted or reflected depends on the initial position of the particle. If the well-posedness criterion would apply then there should also be an initial position for which the particle is trapped inside the well. Note however that trajectories through points where the wave function is zero at the moment that the particle passes are forbidden, because $P(x,t) = 0$ whenever $\psi(x,t) = 0$. The peaks in the quantum potential usually occur where the wave function is zero. Dewdney and Hiley have calculated the possible trajectories for this case numerically and claim to observe what they call a bifurcation effect between the transmitted and reflected trajectories. Let us quote from their paper [DH82]:

"In Fig. 10 we have chosen to explore more trajectories that have initial positions in the front half of the wave packet. All of these are, in fact, transmitted because the particles reach and enter the well before the oscillations in the quantum potential have sufficient energy to change the particle trajectories. The particles whose initial positions lie on the tail side of the center of the packet spend more time in the well as these particles begin to encounter the oscillation in the quantum potential. This has the effect of spreading out the emerging trajectories which form the tail of the transmitted packet.

We have increased the density of trajectories between the initial positions 0.47 and 0.46 so that the region of bifurcation that occurs between these limits could be more clearly shown. The trajectory from 0.47 reaches the peak in the quantum potential at the front of the well with enough energy to traverse it and enter the well. The trajectory from 0.46, however, being further in the tail of the packet, experiences a greater deceleration from the initial inverse parabola formed by the quantum potential. This, coupled with the fact that it reaches the same peak at a slightly later time when its magnitude is greater, ensures that the particle will be reflected.

If we examine more closely the trajectories between 0.47 and 0.46 we see that those that enter the well may be reflected out again because the peaks in the quantum potential in this region are now sufficiently high to repel the particles. These particles actually spend a short time in the well before being ejected to form the tail of the reflected packet."

If this were true then after a certain (bounded) time the probability to find the particle inside the well would have become exactly zero, and there would be no metastable behaviour. A weak point is that their claim is based on numerical analysis. The sharp edges that can be seen in their plot of the quantum potential may well be the result of the finite difference method they use. We saw above that the quantum potential may have sharp edges in principle (like the top of the roof), but in practice wave functions are well-behaved, i.e. infinitely many times differentiable almost everywhere except at the sources of the classical potential (the nucleus of the hydrogen atom is the source of the coulomb force acting on the atom's electron for instance). For a well-behaved wave function interesting behaviour can only be expected at it's zero's, because it's modulus must be differentiated to obtain the quantum potential. Suppose at a certain time t we have $\psi(x,t) = 0$ in $x = 0$ and that the real and imaginary part of the wave function may be expanded in powers of x in the neighbourhood of the origin. Since $|\psi(x)| = \sqrt{\Re^2(\psi(x)) + \Im^2(\psi(x))}$ (ignoring the

t-dependence for the time being), $|\psi|$ may then be expanded in powers of x as well if we take care of the sign of x. For example, for $x \to 0$ we may write

$$
\begin{aligned}
\sqrt{x^2 + x^3 + x^4} &= \pm x \sqrt{1 + x + x^2} \\
&= \pm x (1 + \tfrac{1}{2}x + O(x^2)) \\
&= \pm (x + \tfrac{1}{2}x^2 + O(x^3))
\end{aligned}
$$

where the $+$-sign holds for positive and the $-$-sign for negative values of x. The derivative of the quantum potential with repect to x is given by (apart from an irrelevant constant):

$$
\frac{d}{dx}\left[\frac{|\psi|''}{|\psi|}\right] = \frac{|\psi| \cdot |\psi|''' - |\psi|'' \cdot |\psi|'}{|\psi|^2}
$$

Using the expansion of $|\psi|$ in powers of x we see that the lowest power of x in the denominator must be even. In order to have a roof-like quantum potential with it's top in $x = 0$, the derivative should change it's sign there. This means that the lowest power of x in the numerator should be odd. Hence, the roof is either completely flat (if the lowest power of x in the numerator is larger than in the denominator) or an infinite spike. In the latter case the quantum potential has a singularity in $x = 0$. Consider for instance $\psi(x) = ax^2 + bx^3$, with a and b larger than zero. We then have

$$
\frac{|\psi|''}{|\psi|} = \frac{2a + 6bx}{ax^2 + bx^3} \to \infty \quad \text{if } x \to 0
$$

and

$$
\frac{d}{dx}\left[\frac{|\psi|''}{|\psi|}\right] \to -\frac{4}{x^3} \quad \text{if } x \to 0
$$

At a slightly earlier moment in time the wave function may be given by $\psi(x) = c + ax^2 + bx^3$ with a very small positive constant c. The quantum potential in the origin is then equal to $\frac{2a}{c}$ and it's derivative equal to $\frac{6b}{c}$. So at the moment that c becomes zero the quantum potential and it's derivative in the origin change discontinuously.

Whether this is enough to explain the bifurcation effect of Dewdney and Hiley remains to be seen. They may be wrong after all. On a priori grounds we cannot see that they are, however. We should treat this as an open question that can only be answered by further research. By the same token we feel that Marino and others have no ground to suppose that the well-posedness criterion applies to all physical systems. The unavoidability of metastable behaviour in bistable physical systems should therefore also be treated as an open question.

Acknowledgements

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