Transition to Localization of Biased Walkers in a Randomly Absorbing Environment

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We study biased random walkers on lattices with randomly dispersed static traps in one, two and three dimensions. As the external bias is increased from zero the system undergoes a phase transition, most clearly manifested in the asymptotic drift velocity of survivors which is zero below a critical bias. This transition is second-order in one dimension but of first order in higher dimensions. The model can be mapped to a stretched polymer with attractive interaction between monomers, and this phase transition would then describe sudden unfolding of the polymer when the stretching force exceeds a critical value. We also present precise simulations of the zero bias case where we show unambiguously that the transition between the Rosenstock and Donsker-Varadhan regimes is first order in dimension $\geq 2$.

I. INTRODUCTION

The behavior of a particle diffusing amidst randomly dispersed static traps is already interesting by itself, but also because of its connections to several other problems: It is closely related to the Anderson model of delocalization and to some models of population dynamics \cite{1}. It can be mapped exactly onto flux lines in a medium with parallel columnar defects \cite{1} and to the collapse of a self-attracting polymer without excluded volume interaction.

The problem is usually formulated as a random walk on a $d$-dimensional lattice; a random fraction $c$ of all lattice sites is occupied by traps which kill a walker if it happens to land on them. The main quantity of interest is the survival probability after $t$ steps, $P(c,t)$, averaged over all walks and all trap configurations. For small $t$ and small trap concentrations, $P(c,t)$ decays exponentially as predicted by Rosenstock (RS) \cite{2}, but at later times it crosses over to the exact Donsker-Varadhan (DV) form \cite{3,4}.

$$\ln P(c,t) \sim -A_d \lambda t^{\frac{d}{d+2}}$$

(1)

where $\lambda = -\ln(1-c)$ and $A_d$ are exactly known numerical constants. Eq.(1) can be understood in terms of contributions from large trap-free regions. Such regions are very rare, but survival is much enhanced in them. Thus, $P(c,t)$ is dominated by regions whose size grows with $t$ as $R \sim t^{\frac{d}{d+2}}$ \cite{3,4}.

The precise form of this crossover has been a matter of some controversy \cite{3,4}. In particular, simulations have been notoriously difficult for $d \geq 2$. While deviations from the RS prediction are easily seen \cite{3}, it has proven difficult to access the validity of Eq.(1) in simulations \cite{5,6}. For $d = 3$, the situation has largely been clarified by simulations of Anlauf \cite{10} which unfortunately were never published, and by analytical work by Nieuwenhuizen \cite{9}. Very recently, similar scaling was found in \cite{11,12} to hold also for $d = 2$.

In this paper we first present further simulations of this model where we correct some previously made claims and verify the prediction of \cite{1} that the RS-DV crossover is akin to a first order phase transition at infinite temperature. We then show results of the model with a superimposed bias. In the latter, the jumping rates in the (fixed) bias direction are enhanced by a factor $b > 1$ and those in the opposite direction are suppressed by the same factor.

This external bias leads to a phase transition in the asymptotic dynamics. For small bias the long time dynamics is similar to the zero-bias case: the walkers stay in large trap-free regions and do not drift. Instead, their typical positions increase slowly as $x \sim R \sim t^{1/(d+2)}$. But above a critical bias $b_c$, the surviving walks drift with a finite velocity \cite{3}. These behaviors are separated by a sharp transition which is of second-order in $d = 1$ but of first order in $d \geq 2$. At $b > b_c$ the drift velocity tends to zero in $d = 1$ but reaches a non-zero value $v_\infty$ in $d \geq 2$.

Asymptotically the survival probability decays exponentially in both phases, but the decay rate is singular at the transition point: its slope is discontinuous in $d \geq 2$ while in $d = 1$ the second derivative is discontinuous.

The averaging over disorder can easily be done exactly and leads to

$$P(c,t) = e^{-\gamma t(2d)^{-1}} Z_t$$

(2)

with

$$Z_t = \sum_{\text{walks}} (1-c)^s b^x.$$

(3)

Here,

$$\gamma = \ln\left(\frac{b+b^{-1}-2}{2d} + 1\right)$$

(4)

and $s$ is the number of distinct sites visited. Finally, $Z_t$ can be understood as the partition sum of a self-attracting polymer (without excluded volume interaction; we assume $k_BT = 1$) of length $t$, stretched by applying opposite forces $\pm \ln b$ to its two ends. The self attraction comes about by the fact that each monomer which is placed on a new site is punished by a Boltzmann factor $1 - c$, while no such factor is applied when a monomer...
is placed at a site which is already occupied by another monomer.

Although this is rather artificial as a polymer model, the mapping is very useful for suggesting efficient simulation methods and for interpreting the results.

Our simulations are performed using the Pruned-Enriched-Rosenbluth Method (PERM) [14] which is a growth scheme to build weighted walks: Walks with too small weights are pruned, promising configurations are used to simulate efficiently a large number of polymer problems including Θ-collapse, DNA denaturation, protein folding, and critical unmixing [15]. In addition to the “population control” provided by cloning and pruning, walks are also guided by assigning different a priori probabilities to different jumps. In particular, we chose these such that previously unvisited sites are unfavorably against previously visited ones, \( p_{\text{unvisited}} = (1 - c)p_{\text{visited}} \), and jumps in the bias direction are more likely than others, \( p_{+x} : p_{-x} : p_{\perp} = \sqrt{b} : \sqrt{1/b} : 1 \). These a priori biases are of course compensated by appropriate weight factors \( \propto 1/p \).

II. UNBIASED WALKERS

For \( b = 1 \) walks are asymptotically subdiffusive or localized; the DV theory predicts the mean squared displacement to be \( \langle R^2 \rangle \sim t^{2/(d+2)} \). However, for small trap concentrations walks are brownian at small times \( \langle R^2 \rangle \sim t \) reverting to DV scaling asymptotically from above [10]. This curious nonmonotonicity (also observed in other models of polymer collapse [16,14,17]) results because the most successful walks at shorter times do not survive for longer periods where DV scaling holds (Fig. 1a). The same is seen, albeit much less dramatically, in \( d = 2 \) (Fig. 1b). It is not seen in \( d = 1 \) where walks remain localized for all times and \( \langle R^2 \rangle \) is monotonic.

![Figure 1](image1)

**FIG. 1.** (a) \( \langle R^2 \rangle \) vs \( t \) in \( d = 3 \) for unbiased walks, showing the sudden localization indicated by the drop in \( \langle R^2 \rangle \). The time at which this localization occurs decreases with increasing trap concentration. The transition proceeds more gradually for larger \( c \), and for \( c > 0.7 \) no maximum is. (b) Similar data for \( d = 2 \). The collapse is there much less pronounced.

The sharp collapse in \( d = 3 \) suggests that the RS-DV crossover is indeed a first order phase transition in the limits \( t \to \infty \) and zero trap concentration, as predicted in [10]. In the polymer model, it would be a first order transition at infinite temperature. A more direct support of this is provided by histograms of the distribution of visited sites. For a first order transition we expect two peaks for large \( t \), the positions of which are separated by a distance \( \propto t \). This is indeed seen in \( d = 3 \) (Fig.2), but not for \( d = 2 \). The latter is not surprising in view of the much softer collapse in \( d = 2 \). It could just mean that the two-peak structure develops only for \( t \) values beyond those obtainable by our simulations (\( t \approx 10^5 \)).

Combining the RS and DV limits into a single scaling ansatz, Anlauf [10] suggested for \( d = 3 \) that the average number of visited sites scales as

\[
\langle s \rangle \sim g_3(\lambda t^{2/3})
\]

A similar ansatz was made for \( d = 2 \) in [11], but as shown in [12] the proper ansatz for \( d = 2 \) must involve logarithmic corrections,

\[
\langle s \rangle \ln t = g_2(\lambda t^{1/2} / \ln t)
\]

As seen from Fig.3a, Eq.(3) does not hold with the simple scaling function proposed in [10]. Anlauf’s data had suggested a piecewise linear \( g_3(x) \) on a log-log plot, with \( g_3(x) = \text{const} \) for \( x < x^* \) and \( g_3(x) = \text{const} / x^{2/5} \) for \( x > x^* \). We see instead from Fig.3a that \( g_3(x) \) develops a kink with infinite slope at \( x = x^* \). This is not too surprising. While a behavior as claimed in [10] would be natural for a second order transition, a more singular behavior is expected for a first order transition. For \( d = 2 \) the scaling function is much smoother (see Fig.3b),
although this might be a transient effect only. We finally point out that we require the precise asymptotics for 2d random walks as derived in [15], with $\ln t$ replaced by $\ln(8t)$, to obtain a good data collapse.

Using Eq. (3), Anlauf had proposed a similar scaling for $P(c, t)$,

$$t^{-1/3} \ln P(c, t) = f_3(\lambda t^{2/3}).$$

Using his simple $g_3(x)$ he derived, by thermodynamic integration, an $f_3(x)$ which gave a very slow convergence to the asymptotic DV scaling after having deviated sharply and suddenly from RS behavior. Although we disagree with his scaling function, our results for $P(c, t)$ (Fig. 4a) fully confirm with his predictions within the numerical errors. Notice that this disagrees slightly with the results found in [12]. Again the analogous ansatz for $d = 2$ should involve logarithms [12], and for a faster convergence we must replace $\ln t$ by $\ln(8t)$,

$$\ln P(c, t)/\ln(8t) = f_2(\lambda t^{1/2}/\ln(8t)).$$

Agreement with simulations is very good, and again we see very slow convergence to the DV asymptotics, in contrast to [12].

III. NONZERO BIAS

For any nonzero bias the long time probability decay is exponential [23]. This is most easily seen as follows: Let $\phi(x, x_\perp, t; b; C)$ be the probability density, for any fixed trap configuration $C$ and bias $b$, that a walker who started at $t = 0$ in the origin $x = 0$ is at time $t$ at the position $x = (x, x_\perp)$. One verifies easily that this is related to the analogous distribution of the bias-free case by (see [21] for the continuum case)

$$\phi(x, x_\perp, t; b; C) = e^{-\gamma t} b^{1/2} \phi(x, x_\perp, t; 1; C).$$

This ‘gauge transformation’ means in particular that the return probability

$$P_{\text{return}}(t) = \langle \phi(0, 0, t; b) \rangle_C$$

decays exactly as

$$P_{\text{return}}(t) = e^{-\gamma t} P^{(b=1)}_{\text{return}}(t),$$

i.e. as an exponential multiplied by the DV stretched exponential since $P^{(b=1)}_{\text{return}}(t)$ also satisfies the DV estimate up to algebraic factors.

For the survival probability we obtain

$$\ln P(c, t) = \ln P^{(b=1)}(c, t) - \gamma t + \ln (\cosh(\alpha b \ln b))_{\text{walks, } C}.$$  

Since the last term is positive definite, we have the exact inequality $\ln P(c, t) \geq \ln P^{(b=1)}(c, t) - \gamma t$. Moreover, if the walkers stay localized in spite of the bias, $x$ increases sublinearly with $t$ and thus the asymptotic decay rate is

$$\alpha = - \lim_{t \to \infty} \frac{1}{t} \ln P(c, t) = \gamma.$$

(13)
Notice that this is independent of the trap concentration. A smaller decay rate can be obtained only when the walkers drift, but then the chance to hit a trap is finite at any time step, and $P(c,t)$ decays again exponentially. Indeed, in the drifting regime any correlations should be short, and thus both the decay rate and the drift velocity are attained already after a short time.

\[ A. \ d = 1 \]

In one dimension it is possible to derive analytic estimates for the survival probability and the drift velocity of delocalized walks. An exact lower bound on the survival probability in terms of probabilities of large trap-free regions is obtained in a way similar to [4], by estimating the contributions of trap-free regions of length $l$ downstream of the starting point of the walker. Take some positive integer $l$ and consider configurations with no trap in the interval $[0,l]$. We then have

\[ P(c,t) \geq (1-c)^l \ P_l(t) \]  \hspace{1cm} (14)

where the first factor on the rhs. is the probability to find such a gap in the trap configuration, and $P_l(t)$ is the probability to survive in it. The latter can be estimated using Eq.(9), the method of images to incorporate the probability to survive in it. The latter can be estimated using Eq.(9), the method of images to incorporate the boundary conditions at $x = -1$ and $x = l + 1$, and Stirling’s formula. We obtain, up to a constant dependent only on $b$,

\[ \ln P_l(t) \geq l \ln b - \gamma t - \left[ \frac{t + l}{2} \ln(1 + \frac{t}{l}) + \frac{t - l}{2} \ln(1 - \frac{t}{l}) \right]. \]  \hspace{1cm} (15)

The rhs. of Eq.(14) is maximal for $l = l^* \equiv t \ tanh[\ln((1-c)b)]$ when $b > b_c \equiv 1/(1-c)$, and for $l = o(t)$ when $b < b_c$. Thus the decay rate is bounded by $\alpha \leq \gamma - \ln[\cosh(\ln(1-c)b))]$ for $b > b_c$. Actually we claim that this bound is saturated, since it can also be understood as the result of a (non-rigorous) saddle point approximation. Summarizing, we have thus found that the decay rate is equal to $\gamma$ for $b < b_c$ and is given by $\alpha = \gamma - \ln[\cosh(\ln(1-c)b))]$ for $b > b_c$. Similarly, the drift velocity of the survivors, defined as $v = \lim_{t \to \infty} v(t)$, vanishes for $b < b_c$ and is given by $v = \tanh[\ln((1-c)b)]$ for $b > b_c$. In the continuum limit ($c \to 0$, $(1-c)b = finite$) this agrees with \[ \alpha = \frac{1}{2} \left( \frac{1}{b} \right) \] but for finite $c$ it disagrees with \[ \alpha = \frac{1}{2} \left( \frac{1}{b} \right) \]. Thus there is a phase transition at $b = b_c$. It is second order in the sense that $v, \alpha$, and $d\alpha/db$ are continuous at $b = b_c$, while $dv/db$ and $d^2\alpha/db^2$ are discontinuous.

These predictions are fully confirmed by simulations, as seen from Figs.5 and 6. In Fig.5 we see $\ln P(c,t) + \gamma t$ versus $t$ for $c = 0.1$ and for several values of $b$. First of all we see that all curves are above that for $b = 1$, as predicted theoretically. Secondly, we see that all curves for $b \leq 1.11$ become horizontal for $t \to \infty$, in agreement with the prediction $b_c = 1/(1-c) = 1.111 \ldots$. The decay rates obtained from Fig.5 for $b > b_c$ are shown in Fig.6a, together with the theoretical predictions. We see that the transition is indeed smooth, as obtained theoretically. Finally, the drift velocities for $c = 0.1$ are shown

\[ \text{FIG. 5. } \ln P(c,t) + \gamma t \text{ for } d = 1 \text{ and trap concentration } c = 0.1. \text{ Statistical errors are smaller than the thickness of the curves.} \]

\[ \text{FIG. 6. } (a) \text{ Decay rate } \alpha \text{ as a function of bias } b, \text{ for } c = 0.1 \ (d = 1). \text{ For } b \geq 1.2 \text{ the statistical errors are much smaller than the size of the symbols; for smaller } b \text{ there is an increasing systematic uncertainty due to the non-trivial extrapolation for } t \to \infty. \ (b) \text{ Analogous results for the drift velocity. Dashed curves are analytic predictions.} \]
in Fig.6a. Again agreement with theory is perfect. We should add that similar results were also found for other values of \( c \), and that \( \langle x \rangle \) increased always monotonically with \( t \), in contrast to what is found for \( d > 1 \) (see below).

### B. \( d \geq 2 \)

In higher dimensions we don’t have similar analytic results. Moreover, direct simulations of the transition region are very difficult, even with our efficient algorithm. But Eq. (13) together with the expected fast convergence of the decay rate and drift velocity in the delocalized phase allow us, in spite of this difficulty, to compute \( v, \alpha \), and \( b_c \) with very high precision.

In Fig.7 we show the average displacements \( \langle x \rangle \) in \( d = 2 \) against \( t \), for \( c = 1/8 \) and for several values of \( b \). Very similar data are obtained for \( d = 3 \) and for other values of \( c \). Obviously \( b_c > 1.65 \), since for all \( b \leq 1.65 \) the curves decrease after an initial rise \( \langle x \rangle \propto t \). The reason for this non-monotonic behavior is the same as in Fig.1: Walkers who venture far out do better initially, but finally only those win who started in a large trap-free region and stayed in it. From Fig.7 one might guess that \( 1.65 < b_c < 1.7 \), but this would be wrong: Also for \( b = 1.7 \) the curve should bend down ultimately, but this will happen very late (see below) and our algorithm might easily miss it (in the transition region it generates many drifting walks with low weight and only very few compact walks, but these with high weight).

The true transition point can be estimated from the survival probabilities, shown in Fig.8 for \( d = 2 \). Actually, in view of eq. (13) we plot \( \log_P(t) + \gamma t \). For small \( b \) we see curves which follow closely the curve for \( b = 1 \), but are slightly above it. These curves contain a linear part at small \( t \) whose slope decreases and whose length increases with \( b \). The cross-over from this linear part to the part following the DV curve is rather sharp and stays so with increasing \( b \). Since the DV curve is asymptotically flat, this scenario should hold up to the value of \( b \) where the “initial” part becomes horizontal. Beyond that value we are in the drifting phase. Obviously the initial straight parts in Fig.8 correspond precisely to the (transient) drifting phase seen already in Fig.7. Indeed, the cross-overs between the two regimes are at the same positions in Figs. 7 and 8.

This means that \( b_c \) is implicitly given by the condition \( \alpha_{\text{drifting}} = \gamma \), where \( \alpha_{\text{drifting}} \) is the decay rate in the drifting phase. While this phase is asymptotically stable for \( \alpha_{\text{drifting}} < \gamma \), it is only transient for \( \alpha_{\text{drifting}} > \gamma \). Even in the transient regime it can be measured precisely (together with the drift velocity), if this regime lasts long enough. Moreover, the drifting phase exists also for \( b < b_c \) and large \( t \), but is only metastable in this regime. This is clearly seen from histograms of the \( x \)-distribution. In Fig.9 (which refers to \( d = 2 \) and \( c = 1/8 \)) we see clearly two peaks in \( P(x) \), for \( t \geq 900 \). The left peak is at \( x/t \approx 0 \). Indeed, it is slightly to the right of \( x/t = 0 \), but it moves to \( x/t = 0 \) for \( t \to \infty \). It of course corresponds to the localized phase. The right peak is the drifting phase. The fact that these peaks become sharper and move apart with increasing \( t \) shows that the transition is first order. For \( d > 2 \) we expect the transition then to be of first order a fortiori.

Since \( \gamma \) is known analytically, we can locate \( b_c \) by simulations in the delocalized phase alone. This procedure is indicated in Fig.10 where the dashed curve is \( \gamma(b) \) and the various continuous curves are finite-time decay rates obtained from short-time runs with different trap concentrations. The error bars of the latter are much smaller than the size of the symbols. The intersection points give \( b_c \) and \( \alpha_c \) in terms of the trap concentration \( c \).
The scaling behavior for $c \to 0$ is easily obtained by observing that $\gamma \approx (b - 1)^2/(2d)$ for $b \approx 1$, while $\alpha \sim c$ in the drifting phase (see Fig.11). The latter is true for small $c$ since the Rosenstock approximation becomes exact in this limit. Therefore we predict that $b_c - 1 \sim \sqrt{c}$. This is verified in Fig.12 for $d = 2$ and $d = 3$. Finally, from Fig.13 we see that also $v_c \sim \sqrt{c}$, i.e. $v_c \propto b_c$. The latter is very natural, but we must remember that it is not true in $d = 1$.

**FIG. 9.** Histograms of the rescaled end point distance $P(x/t)$ versus $x/t$ for $d = 2$ and $c = 0.125$. Biases were adjusted so that both peaks have equal height: $b = 1.510 \ (t = 900)$, $1.577 \ (t = 1800)$, $1.608 \ (t = 2700)$, $1.628 \ (t = 3600)$. Normalization is arbitrary. The peak at $x/t \approx 0$ is due to the localized phase, the other corresponds to the drifting phase.

**FIG. 10.** Decay rates $\alpha$ measured in the drifting (delocalized) phase, $d = 3$. The dashed curve is the prediction $\alpha = \gamma(b)$ for the localized phase. To the left of this curve, the drifting phase is only transient. In spite of that, $\alpha$ is easily measured with high precision, thus the statistical errors are $\leq 10^{-4}$, much smaller than the symbols.

**FIG. 11.** Log-log plot of the critical decay rate versus $c$. For small $c$, both curves scale $\propto c$.

**FIG. 12.** Log-log plot of the logarithm of the critical bias versus $c$. For small $c$, both curves scale as $\sqrt{c}$.

**FIG. 13.** Log-log plot of the critical drift velocity versus $c$. The latter is very natural, but we must remember that it is not true in $d = 1$. 
IV. ALTERNATIVE INTERPRETATIONS

A. Population Dynamics

Up to now, we dealt with independent walkers. Detailed studies of this model were often criticized on the grounds that the tiny probabilities that obtain in the DV regime render the results physically irrelevant (in the model with bias, probabilities are even smaller). This criticism can be countered by adding autocatalytic particle production (local production of off-springs) [1].

Thus we consider a model where particles can hop, get absorbed when hitting a trap, and can reproduce with some fixed rate \( \sigma \). For simplicity we do not include any interaction between particles, in particular we do not take into account any excluded volume effect or any competition for food or other resources. The only effect of reproduction is then that the average number of survivors at generation \( t \) is \( P(c, t)(1 + \sigma)^t \).

In the bias-free case any non-zero \( \sigma \) will thus lead to an explosion of the population, indicating that the model is basically sick. But in the case with drift a suitably chosen rate \( \sigma \) will lead to either a much reduced decay of the particle number, or even to a stationary population size. In this case the neglect of excluded volume and saturation effects will be much more benign, and the effects studied in this paper might have a bigger chance to be observable in real experiments.

Finally, including excluded volume effects would lead to directed percolation (contact process) in a random medium [2].

B. Stretched Collapsed Polymers

We have already pointed out that \( Z_t \) (Eq.(3)) can be understood as the partition sum of a polymer with self-attraction of strength \( k_B T \lambda \), and stretched by a force \( k_B T \ln b \). The decay rate is then essentially the free energy per monomer in the thermodynamic limit.

The fact that unfolding of a collapsed polymer is a first order transition is well known [24,25]. The coexistence of stretched and coiled phases corresponds to a "tadpole" configuration [26,27] where part of the chain is collapsed and the rest sticks out of the coil, so that the total length \( x \) is equal to some prescribed value. Our finding that the critical bias is \( \propto \sqrt{c} \) means then that the string tension in a tadpole configuration scales, in the limit of a very long chain and close to the collapse point, as the square root of the monomer-monomer attraction strength. This seems to be a new result, and it remains to see whether it holds also for more realistic polymer models.

The main difference to standard polymer models is the fact that we have neglected here excluded volume effects (they have no counterpart in the trap problem). Thus the collapse of the unstretched polymer happens at infinite temperature in the present model. In the standard polymer models with next-nearest neighbor attraction or with three body repulsion the \( \Theta \)-collapse is second order, in contrast to the present model. But the dependence of \( \langle R^2 \rangle \) on chain length is also non-monotonic in \( d \geq 3 \) [16,17]. In \( d = 4 \) the collapse is indeed "quasi first order" [17], and special care is needed to realize that it actually is continuous. We believe that in the present model the transition is truly of first order.

C. Magnetic Flux Lines

A last interpretation is in terms of magnetic flux lines in a type II superconductor with parallel columnar defects [1]. These defects are quenched and randomly distributed. They tend to pin the flux lines, thus preserving superconductivity in the sample. In the unbiased case, the mean orientation of the flux lines is parallel to the defects, caused by a magnetic field in the same direction. The biased case corresponds then to a non-zero angle between the field and the defects. For small magnetic field the flux lines will essentially follow the defects. But above a critical field strength (resp. tilting angle) the average angle between flux lines and defects is non-zero. Our main result is that this transition is first order in the sense that the average angle jumps by a finite amount when passing through the critical field strength. This jump scales as the square root of the defect density.

V. CONCLUSION

Using extensive Monte Carlo simulations by means of the PERM algorithm, we have studied the problem of particles performing unbiased and biased random walks in media with randomly located traps. In the bias free case we find the first clear numeric indication for the first order nature of the Rosenstock - Donsker-Varadhan transition in 3 dimensions. In \( d = 2 \) the situation is less clear, but we showed that also there the transition is rather sharp. When the diffusion is biased, we find a transition from localized to drifting walkers at a critical bias which depends on the trap density. This transition is second order in \( d = 1 \) but first order in \( d \geq 2 \). Combining the simulations with exact analytic estimates we were able to draw the phase diagram with high accuracy.

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