Study of anomalous kinetics of the single-species bimolecular annihilation reaction in the framework of an effective field-theoretic model

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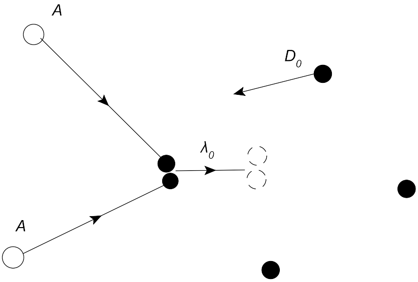
Outline of the presentation

1. Annihilation processes $A + A \to \varnothing$
2. Random velocity fluctuations
3. Master equation approach
4. Field-theoretic model and its RG analysis
5. Main results

Motivation

particles are diffusing with diffusion constant D_0 and reacting after mutual contact



irreversible reaction $A + A \xrightarrow{\lambda_0} \varnothing$

particles A can be interpreted as molecules, biological entities, mutually annihilating random walk etc.

Motivation

- no general theory for non-equilibrium physics
- near critical regimes (phase transitions of 2th order) possible simplifications due to the scale invariance
- reaction processes
  - variety of models can be formulated by the means of reaction processes
    Examples: chemical kinetics, catalysis, spreading of disease, population dynamics, percolation
  - can be analysed by various methods - cellular automata, monte carlo simulations, mapping onto spin systems

Motivation

- we are interested in **approach** to the steady (empty) state from some initial state
- shrinking phase space $\rightarrow$ violation of detailed balance
- determination of possible behaviour (universality classes)
- calculation of critical indices:

  Example: How fast are the particles decaying?

  calculation of decaying exponent α in $n = n(t) \propto t^{-\alpha}$.

reaction limited case...$\tau_{dif} \ll \tau_{react}$

corresponds to high D_0 or small λ_0

no spatial fluctuations $\Rightarrow n = n(t)$

Rate equation $\frac{dn(t)}{dt} = -\lambda_0 n^2(t) \rightarrow n(t) = \frac{n_0}{1+n_0\lambda_0 t}$

for $t \rightarrow \infty$ we have $n(t) \propto t^{-1}$ and n_0 cancel out

diffusion limited case...$\tau_{dif} \gg \tau_{react}$

corresponds to small D_0 or high λ_0

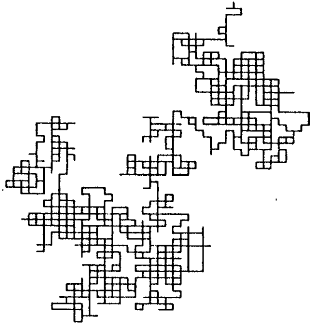
displacement $r(t) \sim (Dt)^{1/2}$

properties of diffusion depends on the value of space dimension d

for $d > 2 \qquad V(t) \sim t$

$n(t)$ should scale as $1/V(t) \rightarrow n(t) \sim t^{-1}$

diffusion for $d \leq 2$ is recurrent $V(t) \sim r(t)^d$



A two-dimensional random walk of 2000 steps.

$$n(t) \sim (Dt)^{-d/2} = (Dt)^{-(1+\Delta)}, \text{ where } d = 2 + 2\Delta$$

Figure from Itzykson& Drouffe: *Statistical Field Theory 1*

Annihilation process in advective environment?

- reactions usually occur in some environment
- this can lead to additional drift of particles
- introduction of $\mathbf{v} = \mathbf{v}(t, \mathbf{x})$ for modelling such situation
- case $\mathbf{v} = \mathbf{v}(\mathbf{x})$ can be interpreted as some kind of disorder
- various origin: thermal fluctuations, external stirring, fluid in turbulent state

Annihilation process in advective environment?

- diffusion - (Peliti 1986), (Lee 1994)
- introduction of velocity fluctuations

$$\partial_t \to \nabla_t = \partial_t + (\mathbf{v}.\nabla),$$
$$n(t) \to \psi(t, \mathbf{x}),$$
$$\partial_t \psi + (\mathbf{v}.\nabla)\psi = D_0 \nabla^2 \psi - \lambda_0 \psi^2$$

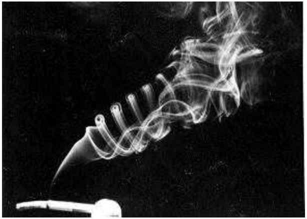
- Does it always enhance the decay process? Can the decay rate be higher than the mean-field rate?

Velocity field

1) stochastic Navier-Stokes equation Monin & Yaglom 1971

- $\partial_t \mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v}$

- control parameter integral-scale Reynolds number $\mathrm{Re} = \frac{L_0 V_0}{\nu}$
  threshold value ($\mathrm{Re} \geq \mathrm{Re}_{crit} \sim 2000$)



- fully developed homogeneous isotropic turbulence (in statistical sense!)
  $\mathrm{Re} \gg \mathrm{Re}_{krit}$, usually $\mathrm{Re} \sim 10^4 - 10^6$

Velocity field

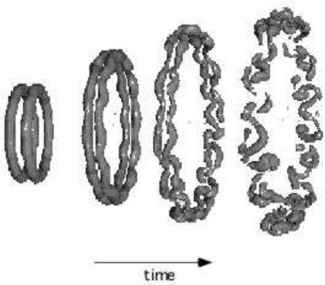
- $\mathbf{v} = \mathbf{v}_{laminar} + \mathbf{v}_{fluctuating}$
- stochastic Navier-Stokes equation for $\mathbf{v}_{fluctuating} \to \mathbf{v}$

$$\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla)\mathbf{v} = \nu \nabla^2 \mathbf{v} - \nabla p + \mathbf{f}^v, \quad (\rho = 1)$$

- random force $\mathbf{f}^v$
  - responsible for stochasticity
  - input of energy to have a steady state
- aim of the theory is to determine scaling behaviour of correlation functions $\langle vv \dots v \rangle$ or response functions $\langle \delta v / \delta f^v \rangle$
- can be considered as microscopic model for turbulence

Velocity field

- 2D turbulence
  - conservation law for enstrophy $\Omega = \langle |\nabla \times \mathbf{v}|^2/2 \rangle$
  - no vortex stretching



- the turbulence in the space dimension $d = 2$ is different from the case $d = 3$ Frisch 1995

Velocity field

2) Let $\mathbf{v}(t,\mathbf{x})$ be a random gaussian field with $\langle \mathbf{v} \rangle = 0$ with second moment

- Kraichnan 1968, Antonov 1999

$$\langle \mathbf{v}_i \mathbf{v}_j \rangle = \int \frac{\mathrm{d}\mathbf{k}\mathrm{d}\omega}{(2\pi)^{d+1}} (P_{ij}^k + \alpha Q_{ij}^k) D_v(\omega, \mathbf{k}) \mathrm{e}^{-i\omega(t-t')+i\mathbf{k}.(\mathbf{x}-\mathbf{x}')},$$

- $P_{ij}^k = \delta_{ij} - k_i k_j / k^2$ - transversal projection operator

- $Q_{ij}^k = k_i k_j / k^2$ - longitudinal projection operator

- by suitable choice of D_v one can get
  (a) rapid-change model (delta correlated in time) $D_v = D_v(\mathbf{k})$ and $\alpha = 0$
  (b) frozen-velocity field $D_v \propto \delta(\omega)$ and $\alpha = 0$
  (c) compressible velocity field $\alpha > 0$, $\nabla.\mathbf{v} \neq 0 \longleftrightarrow \mathbf{k}.\mathbf{v} \neq 0$

Velocity field

$$D_v(\omega, \mathbf{k}) \quad \propto \quad \frac{k^{4-d-2\epsilon-\eta}}{\omega^2 + [u_0 D_0 k^{2-\eta}]^2}$$

ϵ - describes energy spectrum $E(k) \simeq k^{1-2\epsilon}$

η - correlation time t_v of velocity scales as $t_v \propto k^{-\eta+2}$

Kolmogorov regime (turbulent diffusion) obtained for $\epsilon = \eta = 4/3$:

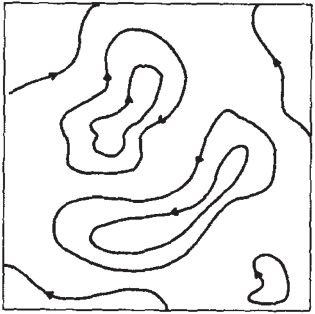
Richardson's law $\langle x^2(t) \rangle \propto t^3$ (superdiffusion)

Five-third's law $E(k) \propto k^{-5/3}$ or $\langle \mathbf{v}(t, \mathbf{r})\mathbf{v}(t, \mathbf{0}) \rangle \propto r^{2/3}$

Frisch 1995

Velocity field

incompressible case



compressible case

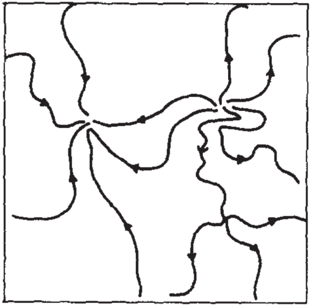
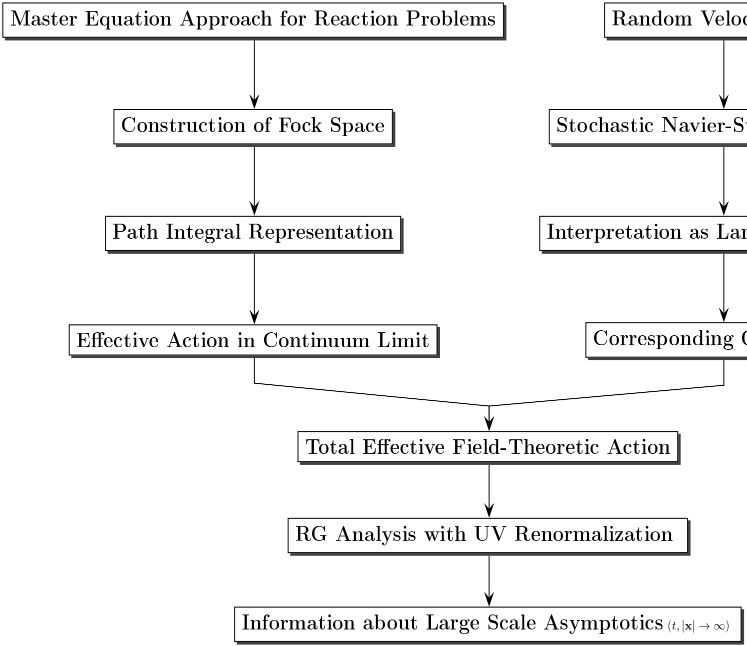


Figure from Bouchaud & Georges 1990

Theoretical model


Master Equation Approach for Reaction Problems
Construction of Fock Space
Path Integral Representation
Effective Action in Continuum Limit
Random Velocity Field
Stochastic Navier-Stokes Equation
Interpretation as Langevin Equation
Corresponding QFT model
Total Effective Field-Theoretic Action
RG Analysis with UV Renormalization
Information about Large Scale Asymptotics $(t, |\mathbf{x}| \to \infty)$

Annihilation process

- particles hopping on a lattice and reacting after contact

- Let $\{\alpha\}$ completely describe microstate, e.g. $\{\alpha\} = \{n_1, n_2, \ldots\}$ means n_1 particles at site 1 etc.

- starting point - master equation

$$\frac{\partial}{\partial t} P(\{\alpha\}; t) = \sum_{\{\beta\}} (R_{\beta \to \alpha} P(\beta) - R_{\alpha \to \beta} P(\alpha)),$$

  where the sum runs over possible microstates β

Annihilation process

- similarities with field theory
  (a) dynamic eq. (master eq.) is linear in time like Schrödinger eq.
  (b) number of particles is changing (like in QFT)

- $\Rightarrow$ indication of possible use of the second quantization method

- **Difference:** intrisic classical stochastic problem, no appearance of $\hbar$

Annihilation process

- based on Doi 1976
- creation-annihilation operators

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0,$$
$$\text{vacuum state } \; |0\rangle : a_i|0\rangle = 0 \text{ for all sites } \; i$$

- state vector

$$|\psi(t)\rangle = \sum_{\{n\}} P(\{n\}; t) a_1^{\dagger n_1} a_2^{\dagger n_2} \ldots |0\rangle$$

- aim is to rewrite the master equation into the Schrödinger-like form

$$\frac{d|\psi\rangle}{dt} = -H|\psi\rangle$$

Annihilation process

- hopping between two sites

$$\frac{d|\psi\rangle}{dt} = D_0(a_2^\dagger - a_1^\dagger)(a_2 - a_1)|\psi\rangle$$

- annihilation at a single site with probability λ_0

$$\frac{dP(n)}{dt} = \lambda_0(n+2)(n+1)P(n+2) - \lambda_0 n(n-1)P(n)$$

- after some algebra

$$\frac{d|\psi\rangle}{dt} = \lambda_0(a^2 - a^{\dagger 2}a^2)|\psi\rangle$$

- together with hopping

$$H = D_0 \sum_{\langle ij\rangle}(a_i^\dagger - a_j^\dagger)(a_i - a_j) - \lambda_0 \sum_i (a_i^2 - a_i^{\dagger 2}a_i^2)$$

Annihilation process

- we are interested in large-scale behaviour
- coherent state representation

$$\hat{a}|\psi\rangle = \psi|\psi\rangle, \quad \langle\psi|\hat{a}^\dagger = \psi^*\langle\psi|\,,$$

- coarse graining procedure

$$\sum_i \to \frac{\int \mathrm{d}\mathbf{x}}{a^d}, \quad \psi_i \to \psi(t,\mathbf{x})a^d, \quad \psi_i^*(t) \to \psi^\dagger(t,\mathbf{x}), \quad n_0 \to n_0 a^d,$$

- continuum action S_1 for $A + A \to \varnothing$ is

$$S_1 = \psi^\dagger[-\partial_t\psi + D_0\nabla^2\psi] - \lambda_0 D_0[2\psi^\dagger + (\psi^\dagger)^2]\psi^2 - n_0\psi^\dagger|_{t=0}$$

- integrations are omitted, e.g. $\psi^\dagger\partial_t\psi = \int \mathrm{d}t\mathrm{d}\mathbf{x}\, \psi^\dagger(t,\mathbf{x})\partial_t\psi(t,\mathbf{x})$

Stochastic dynamics and QFT

$$\partial_t\phi(x) = U(x;\phi) + f(x), \qquad \langle f\rangle = 0, \quad \langle f(x)f(x')\rangle = D(x,x'),$$

where f is Gaussian variable and $U(x;\phi)$ is a given t-local functional not containing time derivatives of ϕ.
This problem is equivalent to the quantum field model with double number of fields $\Phi = (\phi, \phi')$ with action

$$S(\Phi) = \frac{1}{2}\phi' D\phi' + \phi'[-\partial_t\phi + U(\phi)]$$

Janssen 1976, De Dominicis 1978

Field-theoretic model

- for stochastic Navier-Stokes equation (model **1**)

$$S_2 = \frac{1}{2}\mathbf{v}' D \mathbf{v}' + \mathbf{v}'[-\partial_t \mathbf{v} - (\mathbf{v}\cdot\nabla)\mathbf{v} + \nu_0 \nabla^2 \mathbf{v}]$$

Adzhemyan, Vasil'ev, Pis'mak 1983

- Kraichnan-Antonov (model **2**)

$$S_2 = -\frac{1}{2}\,\mathbf{v} D_v^{-1} \mathbf{v},$$

Antonov 1999

Field-theoretic model

- total weighted functional

$$\mathcal{W}[\psi^\dagger, \psi, \mathbf{v}, \mathbf{v}'] = \exp(S_1 + S_2)$$

- can be analyzed by standard field theoretical methods
- Feynman diagrammatic expansion
- it can be shown that model is multiplicatively renormalizable
- perturbative RG approach with the use of minimal subtraction scheme
- calculation of fixed points and determination of stable regimes
- solving Callan-Symanzik equation for $n(t)$

Results for $A + A \to \varnothing$ and stochastic Navier-Stokes eq.

- double expansion in (Δ, ϵ), where $\Delta = (d-2)/2$ is deviation from space dimension 2 and ϵ - deviation from the Kolmogorov scaling
- second moment of force correlator

$$\langle f_m(t, \mathbf{k}) f_n(t', \mathbf{k}') \rangle \propto P_{mn}(\mathbf{k}) \delta(t-t') \delta(\mathbf{k}+\mathbf{k}') d_f(k)$$

- kernel function

$$d_f(k) = d_{f_1}(k) + d_{f_2}(k) = g_{10} \nu_0^3 k^{4-d-2\epsilon} + g_{20} \nu_0^3 k^2$$

- multiplicative renormalization

$$g_1 = g_{10}\mu^{-2\epsilon}Z_1^3, \quad g_2 = g_{20}\mu^{2\Delta}Z_1^3Z_3^{-1}, \quad u = u_0 Z_1 Z_2^{-1},$$
$$\lambda = \lambda_0\mu^{2\Delta}Z_2Z_4^{-1}, \quad \nu = \nu_0 Z_1^{-1}, \quad D = D_0 Z_2^{-1},$$

- μ is mass scale in the MS scheme

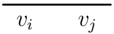
- $u = D/\nu$ is inverse Prandtl number

- RG constants $Z_i, i = 1, 2, 3, 4$ are determined from the UV divergent parts of the 1PI functions $\Gamma_{\psi^\dagger\psi}, \Gamma_{\psi^\dagger\psi^2}, \Gamma_{(\psi^\dagger)^2\psi^2}$, $\Gamma_{\tilde{v}v}$ and $\Gamma_{\tilde{v}\tilde{v}}$.

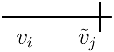
- singularities are realized in the form of poles in ϵ and Δ and their linear combinations such as $2\epsilon + \Delta$ or $\epsilon - \Delta$

- for the consistency of the $\overline{\text{MS}}$ scheme it is necessary that the ratio $\xi = \frac{\Delta}{\epsilon}$ is a finite real number.

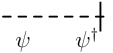
The propagators of the model



$$= \langle v_i v_j \rangle_0 \equiv \Delta^{vv}_{ij}(\omega_k, \mathbf{k})$$

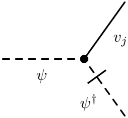


$$= \langle v_i \tilde{v}_j \rangle_0 \equiv \Delta^{v\tilde{v}}_{ij}(\omega_k, \mathbf{k})$$

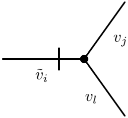


$$= \langle \psi \psi^\dagger \rangle_0 \equiv \Delta^{\psi\psi^\dagger}(\omega_k, \mathbf{k})$$

Interaction vertices describing velocity fluctuation and advection

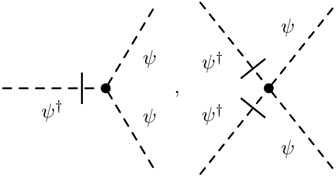


$$\equiv V_j = ik_j$$



$$\equiv V_{ijl} = i(k_j\delta_{il} + k_l\delta_{ij})$$

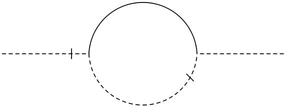
vertices responsible for density fluctuations



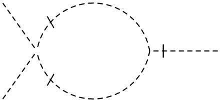
$$\equiv -4\lambda_0 D_0$$

1-loop approximation

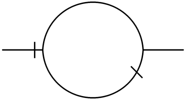
$$\Gamma_{\psi^\dagger\psi} = -DZ_D p^2 +$$



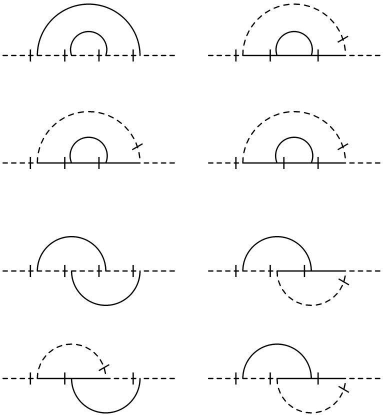
$$\Gamma_{\psi^\dagger\psi^2} = -4D\lambda Z_\lambda \mu^{-2\Delta} + \frac{1}{2}$$



$$\Gamma_{\tilde{v}v} = -\nu Z_\nu p^2 +$$

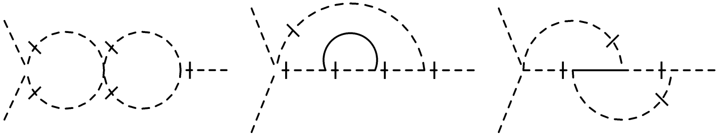


2-loop diagrams for 1PI function $\Gamma_{\psi^\dagger\psi}$

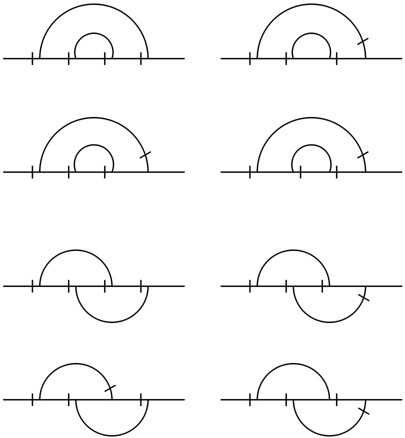


No appearance of reaction vertex $\leftrightarrow$ no feedback from the reaction on the diffusion process

2-loop vertex diagrams



2-loop diagrams for 1PI function $\Gamma_{\tilde{v}v}$



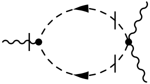
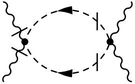
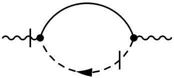
Note: no appearance of diffusion propagator

- Callan-Symanzik equation for the mean particle number

$$\left[(2-\gamma_1)t\frac{\partial}{\partial t}+\sum_g \beta_g \frac{\partial}{\partial g}-dn_0\frac{\partial}{\partial n_0}+d\right]n\left(t,\mu,\nu,n_0,g\right)=0$$

- non-perturbative summation over n_0

- effective action

$\Gamma_R \quad = \quad S_1 + \frac{1}{4}$  $+ \frac{1}{8}$  $+$  $+ \ldots ,$

- stationarity equations

$$\frac{\delta \Gamma_R}{\delta \psi^\dagger}=\frac{\delta \Gamma_R}{\delta \psi}=0$$

- density decay rate $n(t) \propto t^{-\alpha}$
- the decay exponent

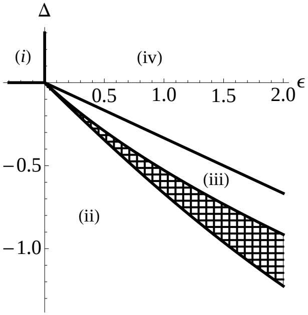
$$\alpha = 1 + \frac{\gamma_4^*}{2 - \gamma_1^*}$$

where the anomalous dimensions γ_2 and γ_4 are defined as

$$\gamma_2 = \left. \frac{\partial \ln Z_2}{\partial \ln \mu} \right|_0, \quad \gamma_4 = \left. \frac{\partial \ln Z_4}{\partial \ln \mu} \right|_0,$$

$$\gamma_2 = \gamma_D, \quad \gamma_4 = \gamma_\lambda - \gamma_D$$

Fixed point[1]	α	region of stability $\mathcal{O}(\epsilon,\Delta)$ [2]
Gaussian (i)	1	$\epsilon<0, \Delta>0$
Thermal (ii)	$1+\frac{\Delta}{2}+\frac{\Delta^2}{2}$	$\Delta<0, 2\epsilon+3\Delta<0$
Anomalous kinetic (iii)	$\frac{1+\Delta}{1-\epsilon/3}$	$\epsilon>0, -2\epsilon/3<\Delta<-\epsilon/3$
Normal kinetics (iv)	1	$\epsilon>0, \Delta>-\epsilon/3$
Driftless (v)	$1+\Delta$	unstable



[1] for $d \le 2$ we have $n(t) \propto t^{-(1+\Delta)}$

[2] quadratic corrections are not presented

(i) Gaussian FP
- stable for $d > 2$ - mean field theory
- needed for the correct use of RG

(ii) Thermal FP
- local correlation stronger than long correlations and because $\Delta < 0$ ineq. $1 + \Delta/2 > 1 + \Delta$ holds
- at thermal point the decay is faster than $n \sim t^{-(1+\Delta)}$

(iii) Normal FP
- stable for $\Delta > -\epsilon/3$ with mean field-like behaviour $\alpha = 1$
- long range correlations destroy any effect of density fluctuations

(iv) Anomalous FP - here we have $1 + \Delta/2 < \alpha = (1 + \Delta)/(1 - \epsilon/3) < 1$

(v) unstable FP - realized when there is no stirring and thermal fluctuations

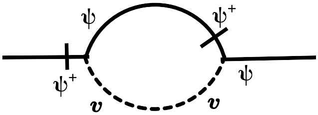
Summary1

- unstable behaviour with respect to the any velocity fluctuations, i.e. thermal fluctuations makes diffusion-caused decay unstable
- mean-field value for the exponent in the basin of attraction of trivial FP and normal FP
- for anomalous FP exact value has been obtained (no correction in ϵ)
- at thermal FP nontrivial correction in ϵ has been obtained

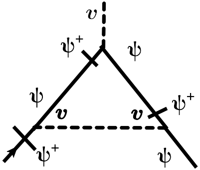
Results for $A + A \to \varnothing$ and Kraichnan model with compressibility

1-loop Feynman diagrams

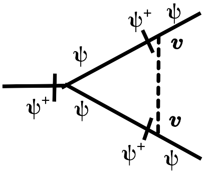
$$\langle \psi^\dagger \psi \rangle_{1-ir} \quad = \quad i\omega - Dp^2 Z_D +$$



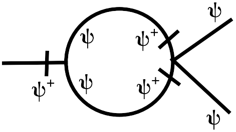
$$\langle \psi^\dagger \psi \mathbf{v} \rangle_{1-ir} \quad = \quad ip_3 Z_{\mathbf{v}} +$$



$$\langle \psi^\dagger \psi^2 \rangle_{1-ir} \quad = \quad -4\lambda D Z_\lambda + \frac{1}{2}$$



$$+ \frac{1}{2}$$



Rapid-change model

$\langle \mathbf{v}(t)\mathbf{v}(t')\rangle \propto \delta(t-t')$

$$g' = \frac{g}{u^2}, \quad w = \frac{1}{u} \Longrightarrow \beta_{g'} = g'[-2\epsilon + \eta + \gamma_D - 2\gamma_{\mathbf{v}}], \quad \beta_w = w[\eta - \gamma_D]$$

condition for this regime $u \to \infty \Leftrightarrow w = 0$
now $n(t) \propto t^{-\beta}$ (because α is reserved for compressibility parameter)

FP	$g^{*\prime}$	λ^*	β	Stable for
1A	0	0	1	$\eta > 2\epsilon, \eta > 0, \delta > 0$
1B	0	$-4\pi\delta$	$1+\delta$	$\eta > 2\epsilon, \eta > 0, \delta < 0$
2A	$\frac{8\pi(2\epsilon-\eta)}{1+\alpha}$	0	$1 + \frac{\alpha}{1+\alpha}\frac{2\epsilon-\eta}{2-2\epsilon+\eta}$	$2\epsilon > \eta > \epsilon, 2\delta > \frac{\eta-2\epsilon}{1+\alpha}$
2B	$\frac{8\pi(2\epsilon-\eta)}{1+\alpha}$	$-4\pi\delta - \frac{2\pi(2\epsilon-\eta)}{1+\alpha}$	$1 + \frac{2\delta+2\epsilon-\eta}{2-2\epsilon+\eta}$	$2\epsilon > \eta > \epsilon, \frac{\eta-2\epsilon}{1+\alpha} > 2\delta$

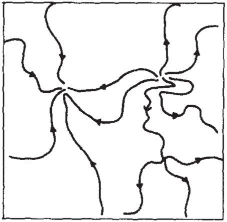
Non-trivial fixed points

for both of them

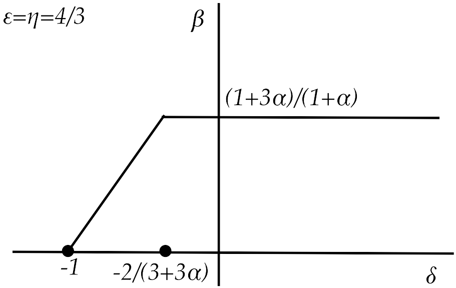
$$\frac{g^*}{8\pi u^*(1+u^*)} = \frac{2\epsilon - \eta}{1+\alpha},$$
$$u^* = -1 + \frac{\alpha(\eta - 2\epsilon)}{(1+\alpha)(\eta - \epsilon)}$$

FP	λ^*	β	Stable for
5A	0	$1 + \frac{\alpha}{1+\alpha}\frac{2\epsilon-\eta}{2-\eta}$	$\epsilon > \eta > \epsilon(1-\alpha), \delta > \frac{2\epsilon\alpha-\eta(1+2\alpha)}{2(1+\alpha)}$
5B	$-4\pi\delta + \frac{2\pi}{1+\alpha}[\alpha\epsilon - \eta(1+\alpha)]$	$1 + \frac{2\delta+\eta}{2-\eta}$	$\epsilon > \eta > \epsilon(1-\alpha), \delta < \frac{2\epsilon\alpha-\eta(1+2\alpha)}{2(1+\alpha)}$

Kolmogorov (turbulent) regime



presence of sinks and sources



Summary 2

- compresibility tends to increase progress of annihilation process
- density fluctuations acts against compresibility
- Kolmogorov regime $\epsilon = \eta = 4/3$ belong to either $5A$ or $5B$ according to the value of δ

  ”critical” value
  $$\delta = -\frac{2}{3(1+\alpha)}$$
  also notice that for 5B choice $\eta = 4/3$ leads to $\beta = 3(1+\delta)$, that is for $\delta = 0$ consistent with Richardson’s law $x^2 \propto t^3$

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Danke für Ihre Aufmerksamkeit

Thank you for your attention