Reaction kinetics in the presence of synthetic velocity field

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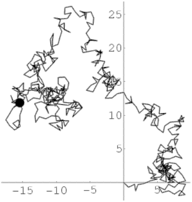
One-species reaction model

- Broad class of chemical reactions $A + A \xrightarrow{\lambda_0} \varnothing$
- Particles constrained to the plane (dimension $d = 2$)
- System is in contact with thermal bath (reservoir) $\rightarrow$ diffusive motion



- Basic questions:
  What is a possible behaviour of the system in IR asymptotics ($t \to \infty$) ?
  What is the value of decaying exponent α, $n(t) \stackrel{t\to\infty}{\longrightarrow} t^{-\alpha}$?

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  1. consider $d \leq 2$, in this case the diffusion is recurrent (Pólya theorem)
     r.m.s. displacement $r(t) \sim (Dt)^{1/2}$ and particles “sweep“ volume
     $V(t) \sim r(t)^d$ completely $\Rightarrow$
     $n(t) \sim (Dt)^{-d/2} = (Dt)^{-(1+\Delta)}$
     deviation from the space dimension $2\Delta = d - 2$

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     deviation from the space dimension $2\Delta = d - 2$
  2. for $d > 2$ $\quad V(t) \sim t \Rightarrow n(t) \sim t^{-1}$

Chemical reaction in turbulent environment?

- Influence of density fluctuations was studied in
  Peliti, J. Phys. A **19**, L365 (1986); B. P. Lee, J. Phys. A **27**, 2633 (1994)
  How do fluctuations of velocity field influence behaviour of the chemical reaction?

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  (b) $\mathbf{v}(\mathbf{x}, t)$ generated by stochastic Navier-Stokes equation

$$\partial_t \mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} = \nu_0\nabla^2\mathbf{v} - \nabla p + \mathbf{f}^v \tag{2}$$

$\mathbf{f}^v$ - random force

Outline of the field-theoretic approach

1. Field-theoretic model for chemical reaction
2. Field-theoretic model for advecting velocity field
3. Models constructed in logarithmic dimension (connection between IR and UV divergences)
4. Applying renormalization group technique
5. Calculation of renormalization constants $\Rightarrow$ beta functions and anomalous dimensions
6. Zeros of beta functions $\Rightarrow$ determination of IR fixed points

Doi approach to the chemical reaction problems

- 'boson'-like operators (no *i* and $\hbar$)

$$[\psi(\mathbf{x}), \psi^\dagger(\mathbf{x}^{'})] = \delta(\mathbf{x} - \mathbf{x}^{'}) \tag{3}$$

$$[\psi(\mathbf{x}), \psi(\mathbf{x}^{'})] = [\psi^+(\mathbf{x}), \psi^+(\mathbf{x}^{'})] = 0 \tag{4}$$

$$\psi(\mathbf{x})|0\rangle = 0, \langle 0|\psi^\dagger(\mathbf{x}) = 0, \langle 0|0\rangle = 1 \tag{5}$$

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$$|\Phi(t)\rangle = \sum_{\{n_i\}} P(\{n_i\}, t)|\{n_i\}\rangle, \quad |\{n_i\}\rangle = \prod_i [\psi^{+}(\mathbf{x}_i)]^{n_i}|0\rangle \tag{6}$$

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- Master equation rewritten in compact (operator) form

$$\frac{\partial}{\partial t}|\Phi(t)\rangle = -\hat{H}|\phi(t)\rangle, \quad \hat{H} = \hat{H}_A + \hat{H}_D + \hat{H}_R \tag{7}$$

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- Discrete model (particles on the lattice) $\overset{\text{Doi formalism}}{\Longrightarrow}$ continuous model
  L. Peliti J. Physique **46**, 1469 (1985)

Doi approach to the chemical reaction problems

- In this formulation mean values could be obtained via

$$\langle A(t)\rangle = \langle 0|\mathrm{e}^{\int d\mathbf{x}}A(\psi^{+}\psi)\mathrm{e}^{-\hat{H}t}|\phi(0)\rangle \tag{8}$$

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- Expectation values $\Rightarrow$ path integral formulation (over classical fields !) (A. N. Vasiliev, *Functional Methods in Quantum Field Theory and Statistical Physics*)

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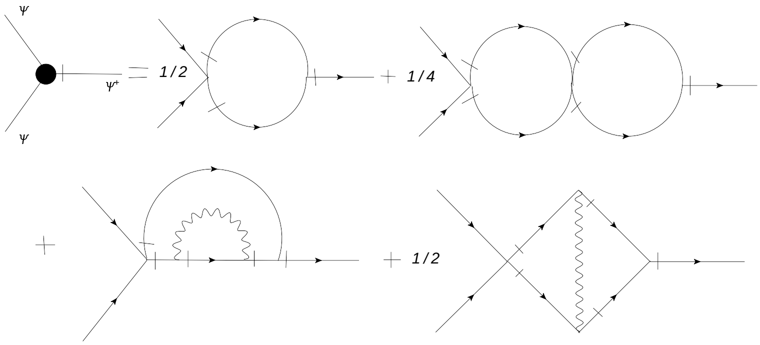
- Action S_1 is given as

$$S_1 = -\int_0^\infty dt \int d\mathbf{x}\,\{\psi^+\partial_t\psi + \psi^+\nabla(\mathbf{v}\psi) - D_0\psi^+\nabla^2\psi + \lambda_0 D_0[2\psi^+ + (\psi^+)^2]\psi^2\} + n_0\int d\mathbf{x}\,\psi^+(\mathbf{x},0) \tag{10}$$

Power counting shows that the model is multiplicatively renormalizable (divergences in $\langle\psi^+\psi\rangle_{\text{1-ir}}$, $\langle\psi^+\psi^2\rangle_{\text{1-ir}}$ and $\langle(\psi^+)^2\psi^2\rangle_{\text{1-ir}}$)



Kraichnan model with finite correlation time

- Describes advection of the passive scalar $\psi(t, \mathbf{x})$

$$\partial_t \psi + (\mathbf{v}.\nabla)\psi = D_0 \partial^2 \psi + f$$

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- Statistical properties are as follows

$$\langle \mathbf{v}(x) \rangle = 0, \qquad \nabla.\mathbf{v} = 0, \qquad m \sim 1/L, \ L - \text{integral scale}$$

$$\langle v_i(x) v_j(x') \rangle = \frac{1}{(2\pi)^d} \int d\mathbf{k}\, P_{ij}(\mathbf{k}) D_v(t - t', k) \mathrm{e}^{i\mathbf{k}.(\mathbf{x}-\mathbf{x}')}$$

$$D_v(t - t', k) = g_0 \frac{D_0^2}{2u_0} \frac{1}{k^{d-2+2\epsilon}} \exp[-u_0 D_0 k^2 (t - t')]$$

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- The total action

$$S = S_1 + S_{\mathbf{v}}$$

where $$S_{\mathbf{v}} = -\int\int d\mathbf{x}dt\, d\mathbf{x}'dt' \frac{\mathbf{v}(\mathbf{x}, t) D_v^{-1} \mathbf{v}(\mathbf{x}', t')}{2}$$

Stochastic Navier-Stokes equations

- Equation for fluctuating part of the velocity field ($\rho = 1$)

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- Random force $\mathbf{f}^v$ responsible for stochasticity and input of energy incompressible fluid $\nabla.\mathbf{v} = 0$ (low Mach number $V_0/V_{sound} \ll 1$)

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- Random force $\mathbf{f}^v$ responsible for stochasticity and input of energy incompressible fluid $\nabla.\mathbf{v} = 0$ (low Mach number $V_0/V_{sound} \ll 1$)
- Action S_{NS} for Navier-Stokes equations

$$\begin{aligned} S_{NS} &= \frac{1}{2}\int dt\, d\mathbf{x}\, d\mathbf{x}'\; \tilde{\mathbf{v}}(\mathbf{x},t).\tilde{\mathbf{v}}(\mathbf{x}',t) d_f(|\mathbf{x}-\mathbf{x}'|) + \\ & \int dt\, d\mathbf{x}\; \tilde{\mathbf{v}}.[-\partial_t \mathbf{v} - (\mathbf{v}.\nabla)\mathbf{v} + \nu_0 \nabla^2 \mathbf{v}] \end{aligned} \tag{12}$$

correlator in the Fourier representation $d_f(k) = g_{10}\nu^3 k^{4-d-2\epsilon} + g_{20}\nu^3 k^2$ (ϵ is a deviation from the Kolmogorov scaling)

Renormalization of the models

- Power counting and analysis of possible divergences
- Both models are multiplicatively renormalizable
- Calculation of the renormalization constants $Z_\alpha \Rightarrow$ beta functions $\beta_g = \mathcal{D}_\mu g$ and anomalous dimensions $\gamma_\alpha \equiv \mathcal{D}_\mu \ln Z_\alpha$, where $\mathcal{D}_\mu = \mu\partial_\mu$
- Fixed points and corresponding critical indices

- In the minimal subtraction scheme with double (ϵ, Δ)-expansion the relations between bare and renormalized paramaters (in MS scheme) are

$$g_{10} = g_1 \mu^{2\epsilon} Z_1^{-3}, \qquad g_{20} = g_2 \mu^{-2\Delta} Z_1^{-3} Z_3,$$
$$\lambda_0 = \lambda \mu^{-2\Delta} Z_2^{-1} Z_4, \quad \nu_0 = \nu Z_1, \quad u_0 = u Z_1^{-1} Z_2$$

- No renormalization of the fields $\psi, \psi^+, \mathbf{v}, \tilde{\mathbf{v}}$ is needed
- Anomalous dimensions $\gamma_a = \mu \frac{\partial \ln Z_a}{\partial \mu}|_0$ and beta functions $\beta_g = \mu \frac{\partial g}{\partial \mu}|_0$, $g = \{g_1, g_2, u, \lambda\}$
- The beta functions could be directly obtained from definition

$$\beta_{g_1} = g_1(-2\epsilon + 3\gamma_1), \qquad \beta_{g_2} = (2\Delta + 3\gamma_1 - \gamma_3)$$
$$\beta_\lambda = \lambda(2\Delta - \gamma_4 + \gamma_2), \qquad \beta_u = u(\gamma_1 - \gamma_2)$$

Fixed points of the model

α - decaying exponent of the particle concentration ($n(t) \propto t^{-\alpha}$)

$$2\Delta = d - 2, \quad \Delta = \mathcal{O}(\epsilon) \Rightarrow \Delta = \xi\epsilon$$
$$\overline{g}^*_\alpha = \overline{g}^*_{\alpha 1}\epsilon + \overline{g}^*_{\alpha 2}\epsilon^2$$
$$\overline{\lambda}^* = \overline{\lambda}^*_1\epsilon + \overline{\lambda}^*_2\epsilon^2$$

Fixed point	α	Region of stability
Gaussian	1	$\epsilon < 0, \Delta > 0$
Driftless	$1 + \Delta$	unstable
Thermal	$1 + \frac{\Delta}{2}$	$2\epsilon + 3\Delta < \frac{3\Delta^2}{2}, \Delta < 0, (R + \frac{1}{2})\Delta^2 > \Delta$
Anomalous kinetics	$\frac{1+\Delta}{1-\epsilon/3}$	$\epsilon > 0, -2\epsilon/3 < \Delta < -\epsilon/3$
Normal kinetics	1	$\epsilon > 0, \Delta > -\epsilon/3$

$R = -0.168$

Conclusions

- Construction of the field-theoretic model of the annihilation reaction $A + A \to \varnothing$
- Calculation of the renormalization constants and RG functions to the two-loop order
- Kraichnan model was studied and compared with the model based on stochastic Navier-Stokes equations
- Callan-Symanzik equation for $n(t) = \langle \psi(t) \rangle$ was solved and decaying exponent at one-loop order was obtained

Thank you for your attention