On the mathematical modelling of the annihilation process

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Mathematical Modelling and Computational Physics
Stará Lesná, 8 July 2011

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Unimolecular reaction model

- Broad class of chemical reactions $A + A \xrightarrow{K_0} \varnothing$
- Particles constrained to the plane (dimension $d = 2$)
- System is in contact with thermal bath (reservoir) $\rightarrow$ diffusive motion and presence of external advecting field (e.g. stirring)
- Basic tasks:
  What is a possible (**stable**) behaviour of the system in IR asymptotics ($t \rightarrow \infty$) ?
  What is the value of decaying exponent α, $n(t) \stackrel{t\rightarrow\infty}{\propto} t^{-\alpha}$?

Unimolecular reaction model

- low probability of K_0 or high mobility of A particles $\rightarrow$
  kinetic rate-equation $\frac{dn(t)}{dt} = -kn^2(t) \rightarrow n(t) \propto t^{-1}$
- experiments, computer simulations, scaling arguments $\rightarrow$
  $n(t) \sim (Dt)^{-d/2} = (Dt)^{-(1+\Delta)}$ for $d < d_c = 2$, where $2\Delta = d - 2$
  with logarithmic corrections for $d = d_c$
  Lee, J. Phys. A **27**, 2633 (1994); Peliti, J. Phys. A **19**, L365 (1986)
- physics od turbulence
  in 2D new conservation law : conservation of vorticity $\boldsymbol{\omega} = \nabla \times \mathbf{v}$ along fluid particle path (when viscosity could be neglected)
  U. Frisch, *Turbulence: the legacy of A.N. Kolmogorov*, Cambridge University Press

Properties of underlying environment

- fluctuating part of the velocity field generated by the stochastic Navier-Stokes equation

$$\partial_t \mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} = \nu_0 \nabla^2 \mathbf{v} - \nabla p + \mathbf{f}, \tag{1}$$

where **f** - random force (energy input and stochasticity)

- properties of the random force

Gaussian variable with zero mean and correlator:

$$\langle f_m(\mathbf{x}_1, t_1) f_n(\mathbf{x}_2, t_2) \rangle = \delta(t_1 - t_2) \int \frac{d\mathbf{k}}{(2\pi)^d} P_{mn}(\mathbf{k}) d_f(k) \mathrm{e}^{\mathrm{i}\mathbf{k}.(\mathbf{x}_1 - \mathbf{x}_2)}, \tag{2}$$

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

where $P_{mn} = (\delta_{mn} - k_m k_n / k^2)$ is transverse projection operator due to the incompressibility condition $\nabla.\mathbf{v} = 0$

- Mean energy input per unit time

$$W = \frac{d-1}{2(2\pi)^d} \int d\mathbf{k} d_f(k) \tag{4}$$

Outline of the field-theoretic approach

1. Classic stochastic problem can be mapped via the Doi approach onto the field-theoretic model
   M. Doi, J. Phys. A **9**, 1465 (1976); **9**, 1479 (1976)
2. Functional formulation
   A. N. Vasiliev, *Functional Methods in Quantum Field Theory and Statistical Physics* (Gordon and Breach, Amsterdam, 1998).
3. Application of robust quantum field methods - perturbative renormalization group
4. Construction and solving of Callan-Symanczik eq. lead to extracting information about infrared (IR) asymptotics, i.e. large space-time scales

Field-theoretic model

- It could be shown (Hnatich and Honkonen PRE **61**, 3904) that

$$\langle A(t)\rangle = \int \mathcal{D}\psi\mathcal{D}\psi^{\dagger} A\{(\psi^{\dagger}+1)\psi\}\exp(S_1) \tag{5}$$

- Action S_1 is given by expression

$$\begin{aligned} S_1 &= -\int_0^{\infty} dt \int d\mathbf{x}\,\{\psi^{\dagger}\partial_t\psi + \psi^{\dagger}\nabla(\mathbf{v}\psi) - D_0\psi^{\dagger}\nabla^2\psi + \\ & \lambda_0 D_0[2\psi^{\dagger} + (\psi^{\dagger})^2]\psi^2\} + n_0\int d\mathbf{x}\,\psi^{\dagger}(\mathbf{x},0) \end{aligned} \tag{6}$$

- Total weight functional could be written as $\mathcal{W}[\psi^{\dagger},\psi,\tilde{\mathbf{v}},\mathbf{v}] = \exp(S_1+S_2)$
- Action S_2 for the Navier-Stokes equation

$$\begin{aligned} S_2 &= \frac{1}{2}\int dt\, d\mathbf{x}\, d\mathbf{x}'\, \tilde{\mathbf{v}}(\mathbf{x},t).\tilde{\mathbf{v}}(\mathbf{x}',t)d_f(|\mathbf{x}-\mathbf{x}'|) + \\ & \int dt\, d\mathbf{x}\, \tilde{\mathbf{v}}.[-\partial_t\mathbf{v} - (\mathbf{v}.\nabla)\mathbf{v} + \nu_0\nabla^2\mathbf{v}] \end{aligned} \tag{7}$$

Field-theoretic model

- UV divergences present at one-particle irreducible (1PI) Green functions $\Gamma_{\psi^\dagger\psi}, \Gamma_{\psi^\dagger\psi^2}, \Gamma_{(\psi^\dagger)^2\psi^2}, \Gamma_{\tilde{v}v}, \Gamma_{\tilde{v}\tilde{v}}$
- Within the means of dimensional regularization the minimal subtraction scheme with double (ϵ, Δ)-expansion gives the following relations between bare and renormalized paramaters

$$
\begin{aligned}
&g_{10} = g_1\mu^{2\epsilon}Z_1^{-3}, \qquad g_{20} = g_2\mu^{-2\Delta}Z_1^{-3}Z_3, \\
&\lambda_0 = \lambda\mu^{-2\Delta}Z_2^{-1}Z_4, \quad \nu_0 = \nu Z_1, \quad u_0 = uZ_1^{-1}Z_2
\end{aligned}
$$

- $u = D/\nu$ is inverse Prandtl number
- Anomalous dimensions $\gamma_a = \mu\partial_\mu \ln Z_a|_0$ and beta functions $\beta_g = \mu\partial_\mu g|_0$, $g = \{g_1, g_2, u, \lambda\}$

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

IR fixed points of the model

- IR asymptotics: small wave vectors **p** and frequencies ω
- Such a behaviour is governed by the IR-stable fixed point $g^* = (g_1^*, g_2^*, u^*, \lambda^*)$: β functions $\beta(g^*) = 0$
- The fixed point g^* is IR stable, if eigenvalues of matrix $\omega_{ij} \equiv \partial\beta_i/\partial g_j|_{g=g^*}$ are positive
- two-loop calculations of 1PI Green functions $\Gamma_{\psi^\dagger\psi}$ and $\Gamma_{\psi^\dagger\psi^2}$
- to the same order of approximation $\Gamma_{\tilde{v}v}$ and $\Gamma_{\tilde{v}\tilde{v}}$ evaluated in L. Ts. Adzhemyan *et al.* Phys. Rev. E **71**, 036305 (2005)
- four IR stable and one unstable fixed point
- **reminder**: $n(t) \sim t^{-\alpha}$ and mean field leads to $\alpha_{mean} = 1$ and $\Delta = \xi\epsilon$ with constant ξ is assumed

(A) The trivial (Gaussian) fixed point

$$g_1^* = g_2^* = \lambda^* = 0, u^* \text{ not determined} \tag{8}$$

$$\epsilon < 0\,, \qquad \Delta > 0\,. \tag{9}$$

$\alpha_G = \alpha_{mean} = 1$

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(B) The short-range fixed point

$$g_1^* = 0\,, \quad g_2^* = -32\pi\Delta + 16\pi(1+2R)\Delta^2,$$
$$u^* = \frac{\sqrt{17}-1}{2} - \pi\Delta^2(Q-\xi),$$
$$\lambda^* = -2\pi\Delta - \pi\Delta^2(Q-\xi), \tag{10}$$

at which local correlations of the random force dominate over the long-range correlations.

$$\Delta - \frac{2R-1}{2}\Delta^2 < 0, \qquad 2\epsilon + 3\Delta - \frac{3\Delta}{2} < 0, \qquad \Delta + \frac{1}{2}\Delta^2 < 0 \tag{11}$$

$\alpha_{short} = 1 + \Delta/2 > 1 + \Delta = \alpha_{fluct}$

α_{fluct} - only density fluctuations

$R = -0.168, Q = 2.64375$

(C) The kinetic fixed point with an anomalous reaction rate:

$$
\begin{aligned}
g_1^* &= \frac{64\,\pi}{9}\,\frac{\epsilon\,(2\epsilon+3\Delta)}{\epsilon+\Delta} + g_{12}^*(\xi)\epsilon^2, \\
g_2^* &= \frac{64\pi}{9}\,\frac{\epsilon^2}{\Delta+\epsilon} + g_{22}^*(\xi)\epsilon^2, \\
u^* &= \frac{\sqrt{17}-1}{2} + u_1^*(\xi)\epsilon, \\
\lambda^* &= -\frac{4\pi}{3}(\epsilon+3\Delta) + \frac{2}{9}(3\Delta+\epsilon)(Q\epsilon-\Delta),
\end{aligned}
\tag{12}
$$

Here $Q = 1.64375$. which is stable, when

$$
\Omega_{\pm} > 0\,, \qquad \epsilon > 0\,, \qquad -\frac{2}{3}\epsilon < \Delta < -\frac{1}{3}\epsilon, \tag{13}
$$

$\alpha_{anom} = (1+\Delta)/(1-\epsilon/3)$

$\alpha_{short} < \alpha_{anom} < \alpha_{mean}$

$$
\begin{aligned}
\Omega_{\pm} \;&=\; \Delta + \frac{4}{3}\epsilon \pm \frac{\sqrt{9\Delta^2 - 12\epsilon\Delta - 8\epsilon^2}}{3} + \frac{2}{9}\Bigg((-3-2R)\epsilon^2 - \\
&\quad 3\epsilon\Delta + \frac{4\epsilon(\epsilon+3\Delta)R - 6\epsilon^2 - 12\epsilon\Delta - 9\Delta^2}{\sqrt{9\Delta^2 - 12\Delta - 8\epsilon^2}}\epsilon\Bigg)
\end{aligned}
\tag{14}
$$

(D) The kinetic fixed point with mean-field-like reaction rate:

$$g_1^* = \frac{64\,\pi}{9}\,\frac{\epsilon\,(2\epsilon + 3\Delta)}{\epsilon + \Delta} + g_{12}^*(\xi)\epsilon^2,$$
$$g_2^* = \frac{64\pi}{9}\,\frac{\epsilon^2}{\Delta + \epsilon} + g_{22}^*(\xi)\epsilon^2,$$
$$u^* = \frac{\sqrt{17} - 1}{2} + u_1^*(\xi)\epsilon\,, \quad \lambda^* = 0\,. \tag{15}$$

This fixed point is stable, when the long-range correlations of the random force are dominant

$$\epsilon > 0\,, \qquad \Delta > -\frac{1}{3}\epsilon\,, \tag{16}$$

and corresponds to reaction kinetics with the normal (mean-field like) decay rate $\alpha_{norm} = 1$

restored mean field like behaviour below $d_c = 2$

(E) Driftless fixed point given by

$$g_1^* = g_2^* = 0, \quad u^* \text{ not fixed}, \quad \lambda^* = -4\pi\Delta, \tag{17}$$

with the following eigenvalues

$$\Omega_1 = -2\epsilon, \quad \Omega_2 = -\Omega_4 = 2\Delta, \quad \Omega_3 = 0. \tag{18}$$

$\alpha_{fluct} = 1 + \Delta$

Conclusions

- The field-theoretic model for the annihilation process $A + A \to \varnothing$ in the presence of advecting velocity field, thermal fluctuations and diffusion motion was constructed
- The renormalization constants and RG functions were calculated to the two-loop order approximation
- Possible IR regimes were obtained together with corresponding regions of stability

Thank you for your attention