# Study of anomalous kinetics of the reaction $A + A \to \varnothing$ to the second order of the perturbation scheme

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# Outline of presentation

- Description of the problem
- Field theoretical model
- Feynman graphs and results
- Conclusions and future work

# Description of the problem

- reaction - diffusion problems $A + B \rightarrow C$
- irreversible process - classical stochastic particle system
- state of the system is far from the equilibrium
- hypercubic lattice $\rightarrow$ continuum limit (Cardy, cond-mat/9607163)
- particles are diffusing all around and react after contact
- in lower dimensions strong dependence of density of reactans on fluctuations $\Rightarrow$ mean-rate equations of little use
- potential applications in chemistry, biology, physics

# Description of the problem

- reaction $A + A \to \varnothing$ as one of the simplest model
- critical dimension of this reaction $d_c = 2$
- advection of reactive scalar by velocity field
- velocity field generated by stochastic Navier-Stokes eqs. with Kolmogorov scaling
- including thermal noise

# Description of the problem

- cast problem into the field theoretic formulation
- employing method of QFT - RG approach
- computation of renormalization constants
- estimating fixed points of RG group
- evaluation of anomalous dimensions and decay rates
- calculation of average number density at one loop level

# Field theoretic model

- we use technique developed by M. Doi (1976) to cast the problem into the quantum field theory language
- details of this technique in M. Doi (J. Phys. A 9, 1465 (1976); 9, 1479 (1976))

this description is based on the use of creation and annihilation operators $\psi$ and $\psi^+$

$$[\psi(\mathbf{x}), \psi^+(\mathbf{x}')] = \delta(\mathbf{x} - \mathbf{x}') \quad (1)$$

$$[\psi(\mathbf{x}), \psi(\mathbf{x}')] = [\psi^+(\mathbf{x}), \psi^+(\mathbf{x}')] = 0 \quad (2)$$

$$\psi(\mathbf{x})|0\rangle = 0, \langle 0|\psi^+(\mathbf{x}) = 0, \langle 0|0\rangle = 1 \quad (3)$$

# Field theoretic model

state vector of many-particle system

$$|\Phi(t)\rangle = \sum_{n_i} P(\{n_i\}, t) |\{n_i\}\rangle \tag{4}$$

basic vectors are traditionally defined as

$$|\{n_i\}\rangle = \prod_i [\psi^+(\mathbf{x}_i)]^{n_i} |0\rangle \tag{5}$$

set of coupled equations for probabilities could be written in the form

$$\frac{\partial}{\partial t} |\Phi(t)\rangle = -\hat{H} |\Phi(t)\rangle \tag{6}$$

where $\hat{H} = \hat{H}_A + \hat{H}_D + \hat{H}_R$

# Field theoretic model

for our problem these terms are given by

$$\hat{H}_A = \int d\mathbf{x} \psi^+ \nabla [\mathbf{v}(\mathbf{x}, t) \psi(\mathbf{x})] \tag{7}$$

$$\hat{H}_D = -D_0 \int d\mathbf{x} \psi^+ \nabla^2 \psi(\mathbf{x}) \tag{8}$$

$$\hat{H}_R = K_{+0} \int d\mathbf{x} (\psi^+)^2 \psi^2 \tag{9}$$

advection, diffusion and reaction part in follow we use definitions

$$\hat{H}'(\psi^+, \psi) = \hat{H}(\psi^+ + 1, \psi) \tag{10}$$

and isolating interaction part

$$\hat{H}'_I = \hat{H}' - \hat{H}'_0 \tag{11}$$

# Field theoretic model

averages are given via the relation

$$\langle A(t)\rangle = \langle 0|T\left(A\{[\psi^+(t)+1]\psi(t)\}\exp(-\int_0^\infty \hat{H}_I' dt + n_0\int d\mathbf{x}\psi^+(\mathbf{x},0))\right)|0\rangle \tag{12}$$

usually initial condition is Poisson distribution

$$|\Phi(0)\rangle = \mathrm{e}^{-\mathrm{n_0 V} + \mathrm{n_0}\int \mathrm{d}\mathbf{x}\psi^+}|0\rangle \tag{13}$$

where $n_0$ is initial number density and $V$ is the volume of the system

# Field theoretic model

by standard procedure (see A. N. Vasiliev, *Functional Methods in QFT and Stat. Phys.*) we could cast (12) it into the functional integral form

$$\langle A(t)\rangle = \int \mathcal{D}\psi^{+}\mathcal{D}\psi A\{[\psi^{+}(t)+1]\psi(t)\}\mathrm{e}^{S_1} \tag{14}$$

where $S_1$ is given by

$$S_1 = -\int_0^{\infty} dt \int d\mathbf{x}\{\psi^{+}\partial_t\psi + \psi^{+}\nabla(\mathbf{v}\psi) - D_0\psi^{+}\nabla^2\psi + \lambda_0 D_0[2\psi^{+} + (\psi^{+})^2]\psi^2 + n_0 \int d\mathbf{x}\psi^{+}(\mathbf{x},0)\} \tag{15}$$

advection velocity field is described by NS eqs.:

$$\partial_t \mathbf{v} + P(\mathbf{v}.\nabla)\mathbf{v} - \mu_0 \nabla^2 \mathbf{v} = \mathbf{f}^v \qquad (16)$$

averaging (14) over random velocity field $\mathbf{v}$

$$\mathcal{W}_2 = \mathrm{e}^{\mathrm{S}_2} \qquad (17)$$

where $S_2$ is action for advection environment

$$S_2 = \frac{1}{2}\int dt d\mathbf{x} d\mathbf{x}' \tilde{\mathbf{v}}(\mathbf{x},t).\tilde{\mathbf{v}}(\mathbf{x}',t) d_f(|\mathbf{x}-\mathbf{x}'|) + \int dt d\mathbf{x} \tilde{\mathbf{v}}.[-\partial_t \mathbf{v} - (\mathbf{v}.\nabla)\mathbf{v} + \nu_0 \nabla^2 \mathbf{v}] \qquad (18)$$

expectation values of any observable could be computed with the use of "complete" weight funtional

$$\mathcal{W} = \mathrm{e}^{\mathrm{S}_1+\mathrm{S}_2} \qquad (19)$$

# Field theoretic model

- two-parameter expansion
- nonlocal term $\Rightarrow$ Kolmogorov scaling (for $\epsilon = 2$)
- local term for RG near $d = 2$ and for generation of thermal fluctuations (Foster, Nelson, Stephen, Phys. Rev. A 16, 732 (1977))

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

correlation function for random force

$$\langle f_m(\mathbf{x}_1, t_1) f_n(\mathbf{x}_2, t_2)\rangle = \delta(t_1 - t_2) \int \frac{d\mathbf{k}}{(2\pi)^d} P_{mn}(\mathbf{k}) d_f(k) \mathrm{e}^{\mathbf{ik}.(\mathbf{x}_1 - \mathbf{x}_2)} \tag{21}$$

$P_{mn} = \delta_{mn} - k_m k_n / k^2$ is the transverse projection operator

# Field theoretic model

renormalized action could be written in the form

$$S = -\int d\mathbf{x}dt\Big\{\psi^+\partial_t\psi + \psi^+\nabla(\mathbf{v}\psi) - u\nu Z_2\psi^+\nabla^2\psi + \lambda u\nu\mu^{-2\delta}Z_4[2\psi^+ + (\psi^+)^2]\psi^2 - \frac{1}{2}\tilde{\mathbf{v}}[g_1\nu^3\mu^{2\epsilon}(-\nabla^2)^{1-\delta-\epsilon} - g_2\nu^3\mu^{-2\delta}Z_3\nabla^2]\tilde{\mathbf{v}} + \tilde{\mathbf{v}}.[\partial_t\mathbf{v} + (\mathbf{v}.\nabla)\mathbf{v} - \nu Z_1\nabla^2\mathbf{v}]\Big\} + n_0\int d\mathbf{x}\psi^+(\mathbf{x},0) \qquad (22)$$

we used abbreviation Prandtl number $u = D/\nu$ and $2\delta = d-2$
$Z_1$ and $Z_3$ are known from two-loops calculations
(Adzhemyan et al. nlin/0207007)
our goal is to determine $Z_2$ and $Z_4$, one loop calculation already done
(Hnatich, Honkonen, Phys. Rev. E 61, 4 (2000))

# Relations for bare and renormalized parameters

$$g_1 = g_{10}\mu^{-2\epsilon}Z_1^3 \tag{23}$$

$$g_2 = g_{20}\mu^{2\delta}Z_1^3 Z_3^{-1} \tag{24}$$

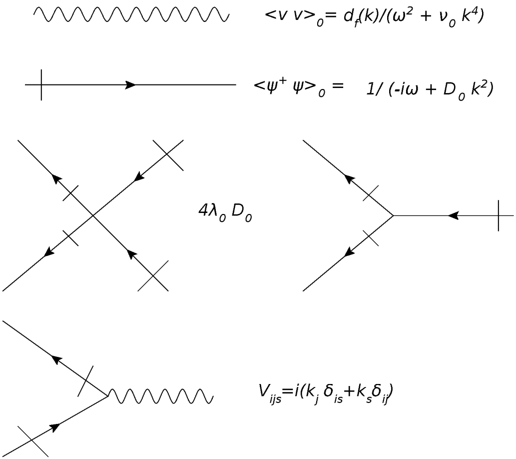
$$\lambda = \lambda_0\mu^{2\delta}Z_2 Z_4^{-1} \tag{25}$$

$$\nu = \nu_0 Z_1^{-1} \tag{26}$$

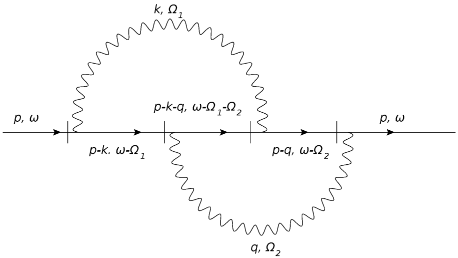
$$u = u_0 Z_1 Z_2^{-1} \tag{27}$$

# Definitions of propagators and vertex factors

from the quadratic part of (18) and (15) follows

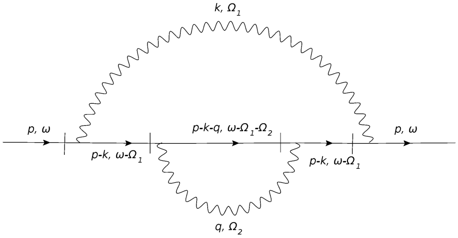


# Two-loops contribution to the $Z_2$




$$\bar{S_d}^2 \frac{d-1}{4d^2(d+2)} \frac{u\nu_0 p^2}{(1+u_0)^4} {}_2F_1\left(1,1,2+\frac{d}{2},\frac{u_0^2}{(1+u_0)^2}\right) \left\{ g_{10}^2 \frac{m^{-4\epsilon}}{4\epsilon} - g_{20}^2 \frac{m^{4\delta}}{4\delta} + g_{10}g_{20}\frac{m^{-2(\epsilon-\delta)}}{2(\epsilon-\delta)} \right\} \quad (28)$$

# Two-loops contribution to the $Z_2$




$$\bar{S_d}^2 \left( \frac{d-1}{d} \right)^2 \frac{\nu_0 p^2}{8(1+u_0)^3} \Big[ A_1 + A_2 + A_3 + A_4 \Big] \tag{29}$$

$$A_1 = g_{10}^2 \frac{m^{-4\epsilon}}{4\epsilon} \left[ -\frac{1}{\epsilon} + \frac{2}{d+2} \frac{u_0^2}{(1+u_0)^2} {}_2F_1 \left( 1, 1, 2 + \frac{d}{2}, \frac{u_0^2}{(1+u_0)^2} \right) \right] \tag{30}$$

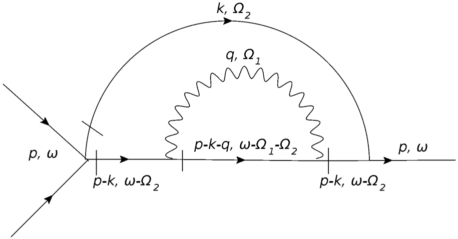
# Two-loops contribution to the $Z_2$

$$A_2 = g_{20}^2 \frac{m^{-4\delta}}{4\delta} \left[ \frac{1}{\delta} + \frac{2}{d+2} \frac{u_0^2}{(1+u_0)^2} {}_2F_1\left(1,1,2+\frac{d}{2},\frac{u_0^2}{(1+u_0)^2}\right) \right] \quad (31)$$

$$A_3 = g_{10} g_{20} \frac{m^{-2(\epsilon-\delta)}}{2(\epsilon-\delta)} \left[ -\frac{1}{\epsilon} + \frac{2}{d+2} \frac{u_0^2}{(1+u_0)^2} {}_2F_1\left(1,1,2+\frac{d}{2},\frac{u_0^2}{(1+u_0)^2}\right) \right] \quad (32)$$

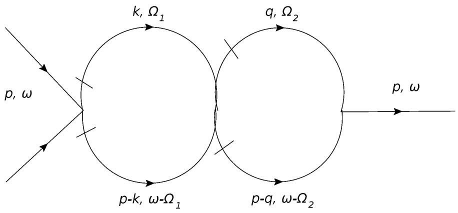
$$A_4 = g_{10} g_{20} \frac{m^{-2(\epsilon-\delta)}}{2(\epsilon-\delta)} \left[ \frac{1}{\delta} + \frac{2}{d+2} \frac{u_0^2}{(1+u_0)^2} {}_2F_1\left(1,1,2+\frac{d}{2},\frac{u_0^2}{(1+u_0)^2}\right) \right] \quad (33)$$

# Two-loops contribution to the $Z_4$



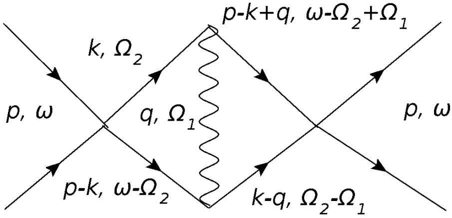

$$\bar{S_d}^2 \frac{d-1}{d} \frac{D_0\lambda_0^2}{u_0(1+u_0)} p^2 \left( \frac{g_{10} m^{-2(\epsilon-\delta)}}{2(\epsilon-\delta)} - \frac{g_{20} m^{4\delta}}{4\delta} \right)$$
$$\left\{ \frac{1}{\delta} + \frac{u_0}{1+u_0} \frac{1}{d+2} {}_2F_1(1,1,\frac{d}{2}+1,\frac{u_0}{2+2u_0}) \right\} \tag{34}$$

# Two-loops contribution to the $Z_4$




$$-\bar{S_d}^2 \frac{D_0 \lambda_0^3}{4} \frac{m^{4\delta}}{4\delta} \tag{35}$$

# Two-loops contribution to the $Z_4$




$$\frac{\bar{S}_d S_{d-1}}{8D_0 u_0^2 (2\pi)^d}\left[\frac{g_{10} m^{-2(\epsilon-\delta)}}{2(\epsilon-\delta)} - \frac{g_{20} m^{4\delta}}{4\delta}\right]\int_{-1}^{1} dz (1-z^2)^{\frac{d-1}{2}}\left[I_{A1}(z) + I_{A2}(z)\right] \quad (36)$$

$$I_{A1}(z) + I_{A2}(z) = \frac{2u_0}{(1-u_0)^2 + 4u_0 z^2} \left\{ \frac{u_0 - 1}{2} \ln \frac{2u_0}{u_0+1} - \frac{2(1+u)_0 z}{\sqrt{1-z^2}} . \left[ \frac{\pi}{2} - \arctan \sqrt{\frac{1+z}{1-z}} \right] + \frac{u_0(u_0+3)z}{\sqrt{2u_0(1+u_0) - u_0^2 z^2}} \left[ \pi - \arctan \frac{zu_0 + u_0 + 1}{\sqrt{2u_0(1+u_0) - u_0^2 z^2}} - \arctan \frac{(2+z)u_0}{\sqrt{2u_0(1+u_0) - u_0^2 z^2}} \right] \right\} \quad (37)$$

# Conclusions

- computation of all two-loops contributions
- complete estimation of $Z_2$ and $Z_4$
- determine fixed points of RG
- add to the model sources and sinks of particles to make the model more general

Thank you for your attention