

Statistical Properties of Random Fields in Stochastic Dynamics and Fully Developed Turbulence

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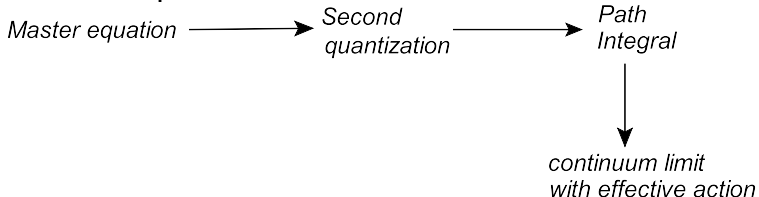
PhD. Defence

Supervised by Michal Hnatič

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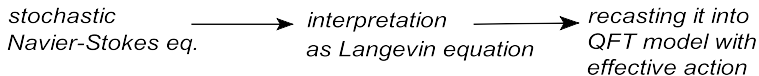
- stochastic dynamics as a part of non-equilibrium physics
- describes large number of phenomena
- there is no general theory for non-equilibrium one
- in critical regimes (second order phase transitions) possible simplifications due to emergent symmetries - scale invariance
- universality
- reaction processes
 - simple formulation
 - can be studied by various methods - cellular automata, monte carlo simulations,
 - genuine in nature: chemical kinetics, catalysis, spreading of disease, population dynamics, percolation etc.

Annihilation process



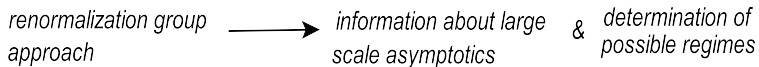
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Random velocity field



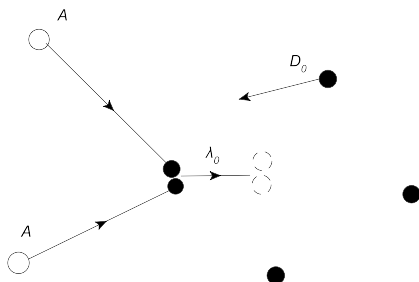
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At the very end



3

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



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

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

corresponds to high D_0 or small λ_0

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

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

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

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

corresponds to small D_0 or high λ_0

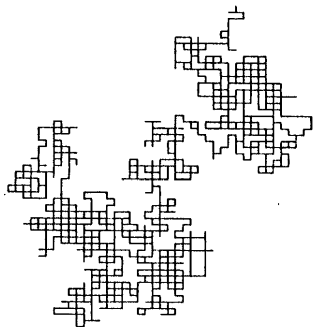
displacement $r(t) \sim (Dt)^{1/2}$

diffusion different in low and high space dimension

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

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

for $d \leq 2$ (diffusion is recurrent¹) $V(t) \sim r(t)^d$



A two-dimensional random walk of 2000 steps.

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

¹fig. from Itzykson& Drouffe: Statistical Field Theory

- 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
- various origin: thermal fluctuations, external stirring, fluid in turbulent state

Various choices for $\mathbf{v} = \mathbf{v}(t, \mathbf{x})$

- 1 Kraichnan model $\mathbf{v}(t, \mathbf{x})$ - random gaussian variable with prescribed statistical properties
 $\langle \mathbf{v}(t) \mathbf{v}(t') \rangle \propto \delta(t - t')$
- 2 Kraichnan model with finite correlation time
- 3 compressible Kraichnan model
- 4 stochastic Navier-Stokes equation $\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{f}$

Questions:

- What is the effect of introduction of velocity field?
- Does it always leads to the enhancement of the reaction process ?
- Quantitatively: what is the value of exponent α in decay $n(t) \propto t^{-\alpha}$?
- What is the effect of velocity field on stability of large scale behaviour?

Theoretical Approach

Reaction processes

- Particles hopping on a lattice and reacting after contact
- Let $\{\alpha\}$ completely describe microstate, e.g. $\{\alpha\} = \{n_1, n_2, \dots\}$ means n_1 particles at site 1 etc.
- starting point - master equation

$$\frac{\partial}{\partial t} P(\{\alpha\}; t) = \sum_{\{\beta\}} (R_{\beta \rightarrow \alpha} P(\beta) - R_{\alpha \rightarrow \beta} P(\alpha)), \quad (1)$$

where the sum is performed over all possible microstates β

- similarities with field theory
 - (a) dynamic eq. (i.e. master eq.) is linear in time like Schrödinger eq.
 - (b) number of particles is changing (like in QFT)
- \Rightarrow suggestion of using second quantization method
- classical stochastic problem, no appearance of \hbar

- based on M. Doi, J. Phys. A **9**, 1465 (1976)
- Introduce creation-annihilation operators

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0, \quad (2)$$

vacuum state $|0\rangle : a_i|0\rangle = 0$ for all sites i

- probability incorporated into the state vector

$$|\psi(t)\rangle = \sum_{\{n\}} P(\{n\}; t) a_1^{\dagger n_1} a_2^{\dagger n_2} \dots |0\rangle \quad (3)$$

- master equation rewritten in "Schrödinger"like form

$$\frac{d|\psi\rangle}{dt} = -H|\psi\rangle, \quad H = H(a^\dagger, a) \quad (4)$$

- "Hamiltonian" for reaction process $A + A \rightarrow \emptyset$

$$H = D_0 \sum_{\langle ij \rangle} (a_i^\dagger - a_j^\dagger)(a_i - a_j) - \lambda_0 \sum_i (a_i^2 - a_i^\dagger{}^2 a_i^2) \quad (5)$$

- Note $H \neq H^\dagger$
 - non-equilibrium theory
 - detailed balance condition not satisfied
 - phase space is shrinking
- possible generalizations to other reaction schemes
U. Täuber *et al.* J. Phys. A: Math. Gen **38**, R79 (2005)

Why continuum limit?

- in statistical physics one often wants to study universal properties in some asymptotic regime
- universal quantities don't depend on the details of microscopic structure or precise value of coupling constant
- Examples: critical exponents
 - (a) critical exponents for φ^4 theory

$$\langle \varphi \varphi \rangle \propto \frac{1}{|\mathbf{r}|^{d-2+\eta}}, \quad M \propto |T_c - T|^\beta, \quad C \propto |T - T_c|^\alpha$$

- (b) for isotropic homogeneous turbulence $\langle (\mathbf{v}(\mathbf{r}, t) - \mathbf{v}(\mathbf{0}, t))^2 \rangle \propto |\mathbf{r}|^{2/3}$

Main result of Doi approach

- using coherent state representation action for process $A + A \rightarrow \emptyset$ is obtained

$$S_1 = \psi^\dagger [-\partial_t \psi + D_0 \nabla^2 \psi - \nabla(\mathbf{v}\psi)] - \lambda_0 D_0 [2\psi^\dagger + (\psi^\dagger)^2] \psi^2 - n_0 \psi^\dagger(\mathbf{x}, 0)$$

- integrations are omitted

$$\psi^\dagger \partial_t \psi = \int_0^{t_f} dt \int d\mathbf{x} \psi^\dagger(t, \mathbf{x}) \partial_t \psi(t, \mathbf{x})$$

- weight e^{S_1} analog to the Boltzmann weight in functional space

Inclusion of velocity fluctuations

- convective derivative $\partial_t \rightarrow \partial_t + (\mathbf{v} \cdot \nabla)$
- for Kraichnan-like model

$$S_2 = -\frac{1}{2} \mathbf{v} D_v^{-1} \mathbf{v}, \quad (6)$$

- stochastic Navier-Stokes eq.

$$S_2 = \frac{1}{2} \mathbf{v}' D \mathbf{v}' + \mathbf{v}' [-\partial_t \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \nu_0 \nabla^2 \mathbf{v}] \quad (7)$$

- averages can be calculated as functional integral

$$A(t) = \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \mathcal{D}\mathbf{v} \mathcal{D}\tilde{\mathbf{v}} A e^{S_1 + S_2}, \quad \mathcal{D}\psi^\dagger \mathcal{D}\psi \dots \Leftrightarrow \text{Tr} \dots$$

Technical details

- Field theoretic action $S_1 + S_2$ is amenable to perturbative RG analysis
- multiplicative renormalization of models
- use of minimal subtraction scheme for calculating renormalization constants Z
- calculation of beta functions β_g and anomalous dimensions γ
- IR stable fixed point determine possible large-scale regime

Interesting Results

Results for $A + A \rightarrow \emptyset$ and stochastic Navier-Stokes eq.

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

$$\langle f_m(t, \mathbf{k}) f_n(t', \mathbf{k}') \rangle \propto P_{mn}(\mathbf{k}) \delta(t - t') \delta(\mathbf{k} + \mathbf{k}') d_f(k) \quad (8)$$

- kernel function

$$d_f(k) = d_{f1}(k) + d_{f2}(k) = g_{10} \nu_0^3 k^{4-d-2\epsilon} + g_{20} \nu_0^3 k^2 \quad (9)$$

- for $d \leq 2$ it was estimated that without velocity field (only diffusion) $n(t) \propto t^{-(1+\Delta)}$

The propagators of the model

$$\overline{v_i \quad v_j} = \langle v_i v_j \rangle_0 \equiv \Delta_{ij}^{vv}(\omega_k, \mathbf{k})$$

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

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

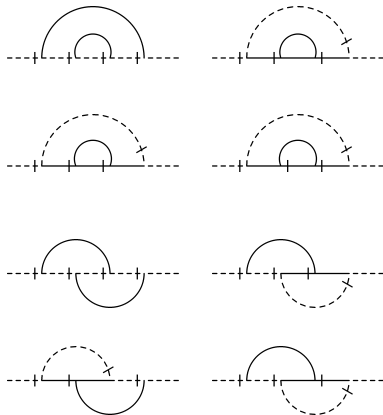
Interaction vertices describing velocity fluctuation and advection

$$\equiv V_j = ik_j$$

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

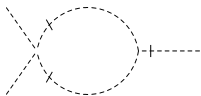
vertices responsible for density fluctuations

$$\equiv -4\lambda_0 D_0$$

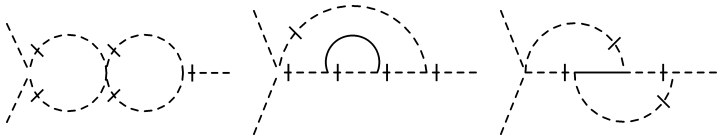
2-loop diagrams for 1PI function $\Gamma_{\psi^\dagger\psi}$ 

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

One loop diagrams for 1PI function $\gamma_{\psi^2\psi^\dagger}$ needed for renormalization of reaction constant λ_0



Second order diagrams



$$\Gamma_R = S_1 + \frac{1}{4} \text{diagram}_1 + \frac{1}{8} \text{diagram}_2 + \text{diagram}_3 + \dots$$

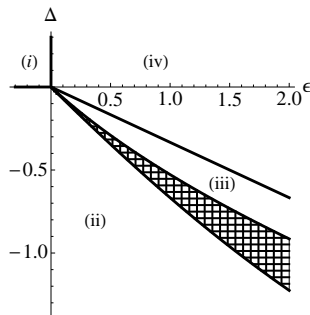
stationarity equations

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

homogeneous case $n = n(t)$

$$\begin{aligned} \frac{dn(t)}{dt} = & -2\lambda u \nu \mu^{-2\Delta} n^2(t) + 2\lambda u \nu \mu^{-2\Delta} n^2(t) \left\{ \frac{\lambda}{4\pi} [\gamma + \ln(2u\nu\mu^2 t)] \right\} \\ & + \frac{\lambda^2 u \nu \mu^{-2\Delta}}{2\pi} \int_0^t dt' \frac{n^2(t') - n^2(t)}{t - t'} \end{aligned} \quad (10)$$

Fixed point	α	region of stability $\mathcal{O}(\epsilon, \Delta)$
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



(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
- so 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 - for it $1 + \Delta/2 < \alpha = (1 + \Delta)/(1 - \epsilon/3) < 1$

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

Summary of our work

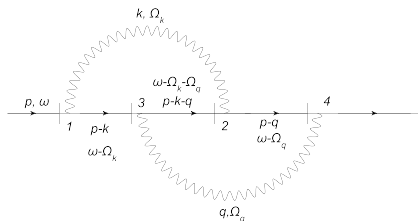
- Kraichnan model (finite correlated in time) + annihilation process
2-loop renormalization
- same model with taken into account of compressibility 1-loop renormalization
- introduction of sink and sources - power counting analysis
- Kraichnan model (finite correlated in time) + percolation

Thank you for your attention

Answers to Prof. Adzhemyan's questions

Q: It is not clear, why the frequency in the formulae (2.16) – (2.18) bears the subscript k (ω_k).

A: The subscript is not necessary in this case. However, in higher order calculations (in our case two loops) one has to deal with two internal momenta - usually denoted as k and q . So the momentum k is associated with frequency ω_k and q with frequency ω_q .



A: mistake in derivation of eq.(3.52), its r.h.s.

$$\exp\left(\sum_i [n_0 \psi_i^*(0) - n_0 - |\psi_i(0)|^2]\right) \rightarrow \exp\left(\sum_i [n_0 \psi_i^*(0) - |\psi_i(0)|^2]\right)$$

then the corrected eq. (3.55) has a form

$$S = \sum_i \left(\psi_i(t) + n_0 \psi_i^*(0) - |\psi_i(0)|^2 - \int_0^t dt [\psi_i^* \partial_t \psi_i + H(\{\psi^*\}, \{\psi\})] \right)$$

and the corrected eq. (3.58)

$$S = - \int_0^t dt \int d\mathbf{x} \left\{ \psi^\dagger \partial_t \psi - D_0 \psi^\dagger \nabla^2 \psi - \lambda_0 [1 - \psi^{\dagger 2}] \psi^2 \right\} + \int d\mathbf{x} \left[\psi(t, \mathbf{x}) + n_0 \psi^\dagger(0, \mathbf{x}) \right]. \quad (11)$$

Now we see that after substitution $\psi^\dagger \rightarrow \psi^\dagger + 1$ the term $\psi(0)$ (from integration) cancels out with the last term n_0 in (11) - in agreement with used initial Poisson distribution.

Q: Akú úlohu hrajú počiatkové podmienky pri hľadaní riešenia? Z účinku vidno, že je narušená translačná invariantnosť, napriek tomu autor používa Fourierovu transformáciu. Môže to zdôvodniť ?

A:

$$\int_0^{\infty} dt \int d\mathbf{x} \psi^\dagger [-\partial_t \psi + D_0 \nabla^2 \psi] + \int d\mathbf{x} n_0 \psi^\dagger(\mathbf{x}, 0) \rightarrow$$

$$\int_{-\infty}^{\infty} \int d\mathbf{x} \psi^\dagger [-\partial_t \psi + D_0 \nabla^2 \psi] + \int d\mathbf{x} n_0 \psi^\dagger(\mathbf{x}, 0)$$

leads to the bare propagator:

$$\langle \psi(\omega', \mathbf{p}') \psi^\dagger(\omega, \mathbf{p}) \rangle_0 \propto \frac{\delta(\omega' + \omega) \delta(\mathbf{p}' + \mathbf{p})}{-i\omega + D_0 p^2} \quad (12)$$

$$\langle \psi(t, \mathbf{p}) \psi^\dagger(0, -\mathbf{p}) \rangle_0 \propto \theta(t) \exp(-D_0 p^2 t) \quad (13)$$

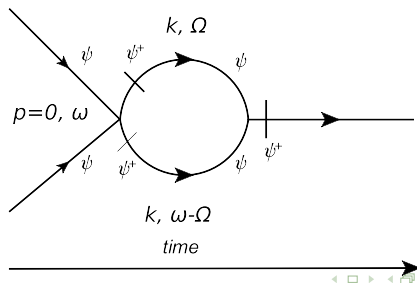
Propagator is **unidirectional** - connects earlier ψ^\dagger with later ψ .

Note there is **no source** of ψ^\dagger field before zero time.

Q: I would also like to see an explanation of the use of the frequency representation in the renormalization of the model with an initial condition.

A:

- Renormalization of the model doesn't depend on the relevant parameter n_0 .
- Consider following diagram - annihilation of two particles



- with the result

$$\begin{aligned} &\propto \int d\Omega d\mathbf{k} \frac{1}{-i\Omega + D_0 k^2} \frac{1}{-i(\omega - \Omega) + D_0(p - k)^2} \\ &\propto \int \frac{d\mathbf{k}}{-i\omega + 2D_0 k^2}, \quad d\mathbf{k} \equiv d^d k \end{aligned}$$

- for $d \geq 2$ UV divergent - not physically interesting, because we know that there should be some cutoff scale
- for $d < 2$ IR divergent, when $\omega \rightarrow 0$ ($t \rightarrow \infty$), connected with reentrant property of random walk in low space dimensions
- RG effectively sums diagrams, which are divergent in the limit $\omega \rightarrow 0$

Answers to Prof. Lisý's questions

Q: Môže sa autor vyjadriť k výberu náhodných zdrojov a absorbérov v 7. kapitole? Je možný ich iný výber? Ak áno, ako ovplyvní tvar účinkov?

A: We have assumed that:

- $A \xrightarrow{\mu^-} X$ and $Y \xrightarrow{\mu^+} A$, X sink, Y source
- μ_{\pm} are random functions uncorrelated in time with moments
 $\mu_{\pm}^n = E_{\pm,n}$
- and taken cumulants only to second order \leftrightarrow normal distribution for μ_{\pm}
- with higher order cumulants continuum limit is not so obvious

Q: Pri poruchových výpočtoch autor používa rozklad podľa voľných parametrov za predpokladu ich malosti. Avšak grafy určujúce oblasti stability pevných bodov (pozri napr. obr.10 str. 68) znázorňujú oblasti obsahujúce aj veľké hodnoty parametrov. Do akej miery je prípustné aproximovať získané výsledky do uvedených oblastí?

A: All the perturbation series are always considered only as **asymptotic** series. However, general expectation is that these series still catch some relevant physics. The situation at the picture should be considered as an extrapolation and also for a better visualization.

Example:

$\mathcal{O}_n \varphi^4$ theory in dimension $d = 4 - 2\epsilon$:

$$\eta = \frac{n+2}{2(n+8)}(2\epsilon)^2 + \frac{(-n^2 + 56n + 272)(n+2)}{8(n+8)^4}(2\epsilon)^3 + \dots \quad (14)$$

Q: Autor uvažuje procesy s rovnakými molekulami. Zrejme interakcie dvoch rôznych molekúl budú patriť do inej triedy univerzality. Predpokladám, že všetok uvedený postup na odvodenie účinku je aplikovateľný aj pre tento proces. Zdalo by sa na prvý pohľad, že spočítať takúto úlohu by už nebol nijaký problém. Alebo sú z fyzikálneho aj technického hľadiska nejaké výrazné problémy, ktoré bránia takému jednoduchému zovšeobecneniu?

A: Yes. $A + B \rightarrow \emptyset$ is in another universality class. It is possible to generalize Doi approach for such a process. Also the renormalization of the model was already performed (see *Lee & Cardy 1994, Honkonen 2002*). The problem is in finding solution for mean particle number. The reason lies in the fact that initial number of particle n_A, n_B are relevant parameters and one has to sum non perturbatively over them.

Q: Autor prezentuje aj partikulárne analytické riešenie (4.66) ním a spoluautormi odvodenej integrálno-diferenciálnej nelineárnej rovnice v hlavnom priblížení podľa väzbovej konštanty λ (zanedbáva integrálny člen). Neskúšal autor hľadať úplné riešenie nezjednodušenej rovnice numericky?

A: To the best of our knowledge, the solution of such equation is not known. But it is our plan for the nearest future to find a solution (most probably using some numerical calculations) without some crude approximation and we would like to try to find solutions, where we could see the effect of the integral term directly.

Answers to Doc. Horváth questions

Q: Ak v rovnici 4.64 položíme $u = 0$, získame tým statické riešenie $n = const$. V prípade $\lambda = 0$ je výsledok nulovania podobný.

A: The parameter is defined as $u = D/\nu$, therefore $u = 0 \rightarrow D = 0$ and hence no movement of reacting particles

The parameter λ (precisely its bare counterpart) is connected with reacting rate of annihilation process, i.e. $\lambda_0 D_0$ is probability per unit time that annihilation process occurs.

Q: Technická a interpretačná vhodnosť iných postupov vedúcich k zavedeniu rýchlostného poľa

1

$$\frac{\partial P_n(t, \mathbf{x})}{\partial t} + (\mathbf{v} \cdot \nabla) P_n(t, \mathbf{x}) = \sum_{\{m\}} R_{m \rightarrow n} P_m(t, \mathbf{x}) - \sum_{\{m\}} R_{n \rightarrow m} P_n(t, \mathbf{x}) \quad (15)$$

2

$$\frac{dn(t)}{dt} = -(K_0 + \eta(t))n^2(t), \quad (16)$$

where $\kappa(t)$ is random variable

3

$$\left[\frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) \right] |\psi(t, \mathbf{x})\rangle = \hat{H} |\psi(t, \mathbf{x})\rangle \quad (17)$$

A: case 1)

- No general prescription for including noise to the master equation
- given equation similar to diffusion equation²

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x_i} A_i(x) P + \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} B_{ij}(x) P \quad (18)$$

substitute $A_i = v_i$ and use $\partial_i v_i = 0$ (incompressible case)

- seems ok

- Possible solution - find hopping rates in proper way³:

$$\frac{\partial P}{\partial t} = \sum_{ij} \left[\tau_{ij}(n_j + 1)P(\dots, n_i - 1, n_j + 1, \dots) - \tau_{ij}n_i P \right] + \dots,$$

$$\frac{1}{\tau_{ij}} = \frac{D}{h^2} [1 + \beta \Delta \mathbf{r} \nabla \times \psi / 2],$$

in such way that we get transport eq. for concentration

$$\frac{\partial c}{\partial t} = D \nabla^2 c - \beta D \nabla \cdot [c \nabla \times \psi],$$

$\beta = 1/(k_B T)$, h lattice spacing, D diffusion, ϕ stream function
 ($\mathbf{v} = \nabla \times \psi$)

³Nga le Tran *et al.* arXiv:cond-mat/9810028

A: case 2)

- Stochastic quantization can be used, but technically it is very difficult.
- in principle solvable, substitution $n(t) = 1/w(t)$

$$\frac{dw}{dt} = K + \eta(t) \Rightarrow w(t) = w(0) + Kt + \int_0^t dt' \eta(t'). \quad (19)$$

From it expectation value of $1/n^2(t)$ can be obtained in some cumbersome form.

- Problem with **physical** interpretation of such a noise. $K + \eta(t)$ as fluctuating rate ? Other than gaussian causes great technical troubles. Here, also large value of η can lead to the $n(t)$ negative!
- maybe better $dn/dt = -Kn(t) + \eta(t)$ with $\langle \eta(t)\eta(t') \rangle \propto n(t)\delta(t - t')$

A: case 3)

- similar to Pauli equation⁴

$$i\hbar\frac{\partial\varphi}{\partial t} = \left[\frac{1}{2m}(\mathbf{p} - e/c\mathbf{A})^2 - \frac{e\hbar}{2mc}\boldsymbol{\delta}\cdot\mathbf{B} + e\Phi \right] \varphi \quad (20)$$

⁴Bjorken&Dreell

Q: Poprosil by som autora dizertácie o vymedzenie osobného podielu na obsahu jeho práce.

A:

- 1 Calculation of renormalization constants for the (Navier-Stokes equation, $A + A \rightarrow \emptyset$) to the second order of perturbation theory. Determination of coordinates of fixed points and their regions of stability.
- 2 Calculation of renormalization constants for the (finite correlated Kraichnan model, $A + A \rightarrow \emptyset$) to the second order of perturbation theory.
- 3 Proposing of the model (compressible Kraichnan model + annihilation process), calculation of renormalization constants (1-loop approx.), determination of fixed points' structure and value of decaying exponent

A:

- 4 Proposing of the model (finite correlated Kraichnan model + directed bond percolation process), calculation of renormalization constants (1-loop approx.-enough for leading contribution of compressibility)
- 5 Preparing manuscripts, conference proceedings and talks on conferences