Master, Fokker-Planck and Langevin equations

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Outline

References

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Outline

1. Introduction
   - Probabilities
   - Probability density function
   - Moments and cumulants
   - Generating functions
     - Moment generating function of a sum
     - Cumulant generating function
   - GAUSSians
   - Central Limit Theorem

2. Stochastic processes

3. Random walks

Probabilities

Basics — Reminders

- $P(\neg A) = 1 - P(A)$
- $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
  $A \cup B$ means that A or B occur (not exclusively), $A \cap B$ means that A and B occur simultaneously.
- $A \cap B = \emptyset$ then A and B are **mutually exclusive**, joint probability factorises
- BAYES's theorem: $P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{P(B|A)P(A)}{P(B)}$

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Probability density function

- **Probability density function** (PDF) $\mathcal{P}_a(x)$ is probability that a is in the interval $[x, x + \mathrm{d}x]$.
- Normalisation: $\int_{-\infty}^{\infty} \mathrm{d}x\, \mathcal{P}_a(x) = 1$
- **Cumulative distribution function** (CDF): $F(z) = \int_{-\infty}^{z} \mathrm{d}x\, \mathcal{P}_a(x)$
- Note: $\mathcal{P}_a(x) = \frac{\mathrm{d}}{\mathrm{d}z} F(z)$
- Extension to joint probability density functions is straight forward.

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Moments and cumulants

- nth moment $\langle x^n \rangle$: $\langle x^n \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\, x^n \mathcal{P}_a(x)$
- **Central moment**: $\langle (x - \langle x \rangle^n \rangle$
- **First cumulant**: $\langle x \rangle_c = \langle x \rangle$
- **Second cumulant**: $\left\langle x^2 \right\rangle_c = \left\langle x^2 \right\rangle - \langle x \rangle^2 = \left\langle (x - \langle x \rangle)^2 \right\rangle = \sigma^2(x)$, the variance.
- In field theory, cumulants correspond to connected diagrams.

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Generating functions

For many problems, generating functions provide a powerful analysis tool. Define the moment generating function (MGF)

$$\mathcal{M}_a(z) = \sum_{i=0}^{\infty} \frac{z^n}{n!} \langle x^n \rangle$$

if the sum converges.

- Note that $\left.\frac{\mathrm{d}^n}{\mathrm{d}z^n}\right|_{z=0} \mathcal{M}_a(z) = \langle x^n \rangle$, *i.e.* differentiation produces the moments.
- By comparison with the definition of an exponential, $\mathcal{M}_a(z) = \langle \exp(xz) \rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \exp(xz) \, \mathcal{P}_a(x)$, the LAPLACE transform of the PDF (characteristic function).

Moment generating function of a sum I

A very useful identity for independent, identically distributed random variables a and b:

$$\mathcal{M}_{a+b}(z) = \ldots = \mathcal{M}_a(z)\,\mathcal{M}_b(z) \quad .$$

Similarly for random variable $y = \alpha x$

$$\mathcal{M}_y(z) = \ldots = \mathcal{M}_x(z\alpha)$$

Note: Every differentiation of $\mathcal{M}_y(z)$ will shed a factor α compared to $\mathcal{M}_x(z)$.

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Cumulant generating function I

Definition of cumulants

Define the cumulant generating function (CGF)

$$\mathcal{C}_x(z) = \ln \mathcal{M}_x(z) \quad ,$$

so that

$$\left.\frac{\mathrm{d}^n}{\mathrm{d}z^n}\right|_{z=0} \mathcal{C}_a(z) = \langle x^n \rangle_c$$

- Zeroth cumulant vanishes, $\ln 1 = 0$, first cumulant is mean $\langle x \rangle_c = \langle x \rangle$.
- Second cumulant is second central moment and thus variance, $\left\langle x^2 \right\rangle_c = \left\langle (x - \langle x \rangle)^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 = \sigma^2(x)$.

Cumulant generating function II

Definition of cumulants

- Third cumulant is the third central moment, $\left\langle x^3 \right\rangle_c = \left\langle (x - \langle x \rangle)^3 \right\rangle$.
- Fourth cumulant and higher: More complicated.
- See skewness and kurtosis.

GAUSSians

GAUSSians are fundamental to all stochastic processes (stability, CLT, WICK's theorem, relation between correlation and independence).

$$\mathcal{G}(x; x_0, \sigma^2) = \frac{1}{\sqrt{2\sigma^2\pi}} e^{-\frac{(x-x_0)^2}{2\sigma^2}}$$

It's straight forward to show that

- $\langle x \rangle = x_0$.
- $\sigma^2(x) = \sigma^2$.
- $\left\langle (x-x_0)^{2n} \right\rangle = \sigma^{2n}(2n-1)!! = \sigma^{2n} 1 \cdot 3 \cdot 5 \ldots (2n-1)$.
- The moment generating function of a GAUSSian is again GAUSSian.
- The cumulant generating function of a GAUSSian is a second order polynomial, $\mathcal{C}_{\mathcal{G}}(z) = zx_0 + (1/2)z^2\sigma^2$.

GAUSSians

The Gaussian solves the diffusion equation

$$\partial_t \phi = D \partial_x^2 \phi - v \partial_x \phi$$

on $x \in \mathbb{R}$, with diffusion constant D, drift velocity v and initial condition $\lim_{t\to 0} \phi = \delta(x - x_0)$. The solution is

$$\phi(x,t) = \mathcal{G}(x - vt; x_0, 2Dt)$$

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Central Limit Theorem I

Consider the "mean"

$$\mathcal{X} \equiv \frac{1}{\sqrt{N}} \sum_{i}^{N} x_i$$

of N independent, identically distributed variables x_i with $i = 1, 2, \ldots, N$ and vanishing mean. The variables themselves have finite cumulants. Note the unusual normalisation $\sqrt{N}^{-1}$.

If the underlying PDF has moment generating function (MGF) $\mathcal{M}_a(z)$, then the MGF of $\mathcal{X}$ is $\mathcal{M}_{\mathcal{X}}(z) = \mathcal{M}_a\left(z/\sqrt{N}\right)^N$ and so the cumulant generating function (CGF) is

$$\mathcal{C}_{\mathcal{X}}(z) = N\mathcal{C}_a\left(z/\sqrt{N}\right) ,$$

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Central Limit Theorem II

so that

$$\left.\frac{\mathrm{d}^n}{\mathrm{d}z^n}\right|_{z=0} \mathcal{C}_{\mathcal{X}}(z) = N^{1-n/2} \left.\frac{\mathrm{d}^n}{\mathrm{d}z^n}\right|_{z=0} \mathcal{C}_a(z) = N^{1-n/2} \langle a^n \rangle_c \ .$$

Thus, all cumulants except the second vanish, the resulting CGF is that of a GAUSSian.

Note what happens if the random variable is not rescaled. In that case cumulants of $\mathcal{X}$ are N times the cumulants of a. This is in sharp contrast to plain moments, which have a much more complicated dependence on N.

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Central Limit Theorem III

The conclusion is the central limit theorem:

Central Limit Theorem (CLT)

The distribution of the random variable

$$\mathcal{X} \equiv \frac{1}{\sqrt{N}} \sum_{i}^{N} x_i$$

based on N independent random variables drawn from them same distribution which has vanishing mean and finite variance tends to a GAUSSian in the limit $N \to \infty$. Extension exist for correlated random variables.

There is a remarkable amount of confusion regarding the rôle of the normalisation by $\sqrt{N}$.

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Central Limit Theorem IV

A GAUSSian is *stable* as the distribution of the sum of to GAUSSian distributed random variables is a GAUSSian again. The same applies to LÉVY distributions.

Outline

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   - Events in time
   - MARKOVian processes
   - CHAPMAN-KOLMOGOROV equations
3. Random walks
4. LANGEVIN equations

Stochastic processes

Mathematicians have a solid definition of a stochastic process.
In the following it is assumed only that

- there is a procedure
- that is not deterministic
- producing a signal (observable)
- as a function of time.

A POISSON process I

A POISSON process is a point process, visualised by points on an interval (think of nails dropped with constant rate on the motorway).

- A configuration are s points on $[0, t]$, say $(\tau_1, \tau_2, \ldots, \tau_s) \in [0, t]^s$ with PDF $Q(\tau_1, \tau_2, \ldots, \tau_s)$.
- The number of points s is itself a random variable.
- Permutations of $(\tau_1, \tau_2, \ldots, \tau_s)$ are the *same* state.
- Permutation π:
  $Q(\tau_1, \tau_2, \ldots, \tau_s) = Q(\tau_{\pi_1}, \tau_{\pi_2}, \ldots, \tau_{\pi_s})$

A POISSON process II

Normalisation:

$$\begin{aligned}
\sum_{s=0}^{\infty} \frac{1}{s!} \int_0^t \mathrm{d}\tau_1 \ldots \mathrm{d}\tau_s \, Q(\tau_1, \ldots, \tau_s) &= \\
\sum_{s=0}^{\infty} \int_0^t \mathrm{d}\tau_1 \int_{\tau_1}^t \mathrm{d}\tau_2 \ldots \int_{\tau_{s-1}}^t \mathrm{d}\tau_s \, Q(\tau_1, \ldots, \tau_s) &= 1
\end{aligned}$$

A POISSON process III

Poisson process

In the POISSON process the PDF factorises and is stationary:

$$Q(\tau_1, \dots, \tau_s) = e^{-\nu(t)} q(\tau_1) \dots q(\tau_s)$$

The normalisation gives $\nu(t) = \int_0^t \mathrm{d}\tau\, q(\tau)$. In the following, the t dependence of ν is dropped.

The probability to find s events within time t is

$$\begin{aligned} \mathcal{P}_P(s) &= \frac{1}{s!} \int_0^t \mathrm{d}\tau_1 \dots \mathrm{d}\tau_s\, Q(\tau_1, \dots, \tau_s) \\ &= e^{-\nu} \frac{1}{s!} \nu^s \ . \end{aligned}$$

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A POISSON process IV

- The average follows as
  $\langle s\rangle = \exp(-\nu)\sum_{s=0}^{\infty}\frac{1}{s!}s\nu^s = \exp(-\nu)\,\nu\sum_{s=1}^{\infty}\frac{1}{(s-1)!}\nu^{s-1} = \nu$.
- The moment generating function follows simply as $\mathcal{M}_P(z) = \exp\left((\exp(z)-1)\langle s\rangle\right)$ and the cumulant generating function is therefore $\mathcal{C}_P(z) = (\exp(z)-1)\langle s\rangle$:

All cumulants $\langle s^n\rangle_c$ with $n \geqslant 1$ are $\langle s\rangle$ in the POISSON process.

- Shot noise (stationary or homogeneous POISSON process): q is constant and $\nu(t) = qt$.
- Probability of no event in $[t, t+\mathrm{d}t]$ is $(1 - q\mathrm{d}t)$ and thus within Δt: $\exp(-q\Delta t)$.
- The probability that an empty interval Δt is terminated by an event is $\exp(-q\Delta t)$ times $\mathrm{d}t\, q$, the probability for an event to take place.

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A POISSON process V

- Also: Probability density for termination of an empty interval:

$$-\frac{\mathrm{d}}{\mathrm{d}\Delta t} e^{-q\Delta t} = q e^{-q\Delta t}$$

i.e. those that terminate do not count in $\exp\left(-q\Delta(t+\mathrm{d}t)\right)$.

Exercise: ZERNIKE's “Weglängenparadoxon”.

Events in time I

- Consider a “random event” x taking place at time t.
- Consider a sequence of random events taking place at *every* point in time.
- $\mathcal{P}_1(x_1, t_1)$ is the probability of observing x_1 at the time (given) t_1 (note: t_1 is *given* and not itself random).
- The joint PDF $\mathcal{P}_2(x_2, t_2; x_1, t_1)$ is the probability to observe x_1 at t_1 and x_2 at t_2.
- Simplify notation by replacing x_i, t_i by i. Also $\mathcal{P}_{n|m}(1, 2, \ldots, n|n+1, \ldots, n+m)$ is the PDF for n events conditional to m.

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Events in time II

- Conditional probability:

$$\mathcal{P}_{1|1}\left(x_2, t_2 | x_1, t_1\right) = \frac{\mathcal{P}_2\left(x_2, t_2; x_1, t_1\right)}{\mathcal{P}_1\left(x_1, t_1\right)} = \frac{\mathcal{P}_{1|1}\left(x_1, t_1 | x_2, t_2\right)\mathcal{P}_1\left(x_2, t_2\right)}{\mathcal{P}_1\left(x_1, t_1\right)} .$$

- **Marginalise over the nuisance variable**:

$$\mathcal{P}_{1|1}\left(3|1\right) = \int \mathrm{d}2\, \mathcal{P}_{2|1}\left(2, 3|1\right)$$

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Events in time III

Since

$$\mathcal{P}_{2|1}(2,3|1) = \frac{\mathcal{P}_3(1,2,3)}{\mathcal{P}_1(1)} = \frac{\mathcal{P}_3(1,2,3)}{\mathcal{P}_2(1,2)} \frac{\mathcal{P}_2(1,2)}{\mathcal{P}_1(1)} = \mathcal{P}_{1|2}(3|1,2)\,\mathcal{P}_{1|1}(2|1)$$

we have

$$\mathcal{P}_{1|1}(3|1) = \int \mathrm{d}2\, \mathcal{P}_{1|2}(3|1,2)\,\mathcal{P}_{1|1}(2|1)$$

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MARKOVian processes I

The term "MARKOVian" refers to the property of a PDF of a time series of events to be conditional only on the latest event. The MARKOVian property depends on the observable chosen:

MARKOV process

The PDF of a MARKOVian process with $t_1 < t_2 < t_3 < \ldots < t_{n+1}$ (for $n \geqslant 1$) has the property

$$\mathcal{P}_{1|n}(n+1|1,2,3,\ldots,n) = \mathcal{P}_{1|1}(n+1|n)$$

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MARKOVian processes II

By Bayes:

$$\begin{aligned}
\mathcal{P}_2(1,2) &= \mathcal{P}_1(1)\,\mathcal{P}_{1|1}(2|1) \\
\mathcal{P}_3(1,2,3) &= \mathcal{P}_2(1,2)\,\mathcal{P}_{1|2}(3|1,2) \\
\mathcal{P}_4(1,2,3,4) &= \mathcal{P}_3(1,2,3)\,\mathcal{P}_{1|3}(4|1,2,3)
\end{aligned}$$

and therefore

$$\begin{aligned}
\mathcal{P}_4(1,2,3,4) &= \mathcal{P}_2(1,2)\,\mathcal{P}_{1|2}(3|1,2)\,\mathcal{P}_{1|3}(4|1,2,3) \\
&= \mathcal{P}_1(1)\,\mathcal{P}_{1|1}(2|1)\,\mathcal{P}_{1|2}(3|1,2)\,\mathcal{P}_{1|3}(4|1,2,3) \ .
\end{aligned}$$

Simplifying the right hand side via the MARKOV property:

$$\mathcal{P}_4(1,2,3,4) = \mathcal{P}_1(1)\,\mathcal{P}_{1|1}(2|1)\,\mathcal{P}_{1|1}(3|2)\,\mathcal{P}_{1|1}(4|3) \ .$$

MARKOVian processes III

Invertibility of the MARKOV property:

$$\mathcal{P}_{1|n}\left(1|2,3,\ldots,n+1\right) = \mathcal{P}_{1|1}\left(1|2\right)$$

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CHAPMAN-KOLMOGOROV equations I

The CHAPMAN-KOLMOGOROV equation are the integral form of the MARKOV property.
The following statement is true *in general*:

$$\mathcal{P}_{1|1}(3|1) = \int d2\, \mathcal{P}_{1|2}(3|1,2)\, \mathcal{P}_{1|1}(2|1)$$

But in case of a MARKOVian process $\mathcal{P}_{1|2}(3|1,2) = \mathcal{P}_{1|1}(3|2)$

CHAPMAN-KOLMOGOROV equation

$$\mathcal{P}_{1|1}(3|1) = \int d2\, \mathcal{P}_{1|1}(3|2)\, \mathcal{P}_{1|1}(2|1)$$

The CHAPMAN-KOLMOGOROV equation is often mis-interpreted as a way of a process “propagating in time” (or “there must be an

CHAPMAN-KOLMOGOROV equations II

intermediate step"). However, this progression is always possible, MARKOVian or not. The CHAPMAN-KOLMOGOROV equation say: In order to propagate, all that is needed is the propagation "matrix" from t_i (initial) to t_f (final): $\mathcal{P}_{1|1}(f|i)$

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Outline

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Random walks

- Consider a sequence of positions $n_0, n_1, n_2, \ldots$ in discrete time $t = 0, 1, 2, \ldots$.
- Continuous version: BROWNian motion.
- Key process in complex systems.

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Pedestrian random walk in discrete time I

Walker starts at time $t = 0$ at position n_0. Position n increases to $n_0 + 1$ with probability p and decreases to $n_0 - 1$ with probability q.
Consider moment generating function of position:

$$\mathcal{M}_{\mathsf{rw}}(z; t = 1) = pe^{z(n_0+1)} + qe^{z(n_0-1)} = \mathcal{M}_{\mathsf{rw}}(z; t = 0)\left(pe^z + qe^{-z}\right)$$

In general, $\exp(zn)$ indicates the position n and its coefficient is its probability.
To evolve the MGF further, in every time step each $\exp(zn)$ is increased to $\exp(z(n+1))$ with probability p and decreased to $\exp(z(n-1))$ with probability q:

$$\mathcal{M}_{\mathsf{rw}}(z; t+1) = \mathcal{M}_{\mathsf{rw}}(z; t)\, pe^z + \mathcal{M}_{\mathsf{rw}}(z; t)\, qe^{-z}$$

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Pedestrian random walk in discrete time II

and therefore

$$\mathcal{M}_{\mathsf{rw}}(z;t) = \mathcal{M}_{\mathsf{rw}}(z;t=0)\left(pe^{z} + qe^{-z}\right)^{t}$$

Explicitly:

$$\mathcal{M}_{\mathsf{rw}}(z;t) = \sum_{i=0}^{t} p^{i} q^{t-i} \binom{t}{i} e^{z(n_0+i-(t-i))}$$

Note parity conservation for even t and inversion for odd t.

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Evolution of the PDF using CHAPMAN-KOLMOGOROV I

Consider the transition matrix

$$\mathcal{P}_{1|1}(x_2, t_2|x_1, t_1) = \frac{1}{\sqrt{4\pi D(t_2 - t_1)}} e^{-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}} ,$$

known as the all-important WIENER process. With an initial δ distribution, the PDF is simply

$$\mathcal{P}_{\text{rw}}(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{(x-x_0)^2}{4Dt}} .$$

Exercise: Show that the Wiener process obeys the CHAPMAN-KOLMOGOROV equation.

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Master equation approach I

Consider the MARKOV property for the **homogeneous** process $T(x_2|x_1; t_2 - t_1) = \mathcal{P}_{1|1}(x_2, t_2|x_1, t_1)$:

$$T(x_3|x_1; \tau + \tau') = \int dx_2\, T(x_3|x_2; \tau')T(x_2|x_1; \tau)$$

where $\tau = t_2 - t_1$ and $\tau' = t_3 - t_2$.
Differentiate with respect to τ' and take $\tau' \to 0$:

$$\begin{aligned}\partial_\tau T(x_3|x_1; \tau) &= \int dx_2\, \big(-a_0(x_2)\delta(x_3 - x_2) + W(x_3|x_2)\big)T(x_2|x_1; \tau) \\ &= \int dx_2\, W(x_3|x_2)T(x_2|x_1; \tau) - a_0(x_3)T(x_3|x_1; \tau)\end{aligned}$$

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Master equation approach II

assuming $\lim_{\tau\to 0} \partial_\tau T(x_3|x_2;\tau) = -a_0(x_2)\delta(x_3-x_2) + W(x_3|x_2)$.
Why does that make sense? Expand T for small τ:

$$T(x_3|x_2;\tau) = (1-a_0(x_2)\tau)\delta(x_3-x_2) + \tau W(x_3|x_2) + \mathcal{O}(\tau^2)$$

and by integrating over x_3:

$$a_0(x_2) = \int \mathrm{d}x_3\, W(x_3|x_2)$$

Master equation approach III

One thus arrives at

Master equation

$$\partial_\tau T(x_3|x_1;\tau) = \int \mathrm{d}x_2 \, \left(W(x_3|x_2) T(x_2|x_1;\tau) - W(x_2|x_3) T(x_3|x_1;\tau) \right) \; ,$$

describing the change of transitions from x_1 to x_3 in time.

If the PDF is known at some time t_1

$$\mathcal{P}_1\left(x_3, t_1 + \tau\right) = \int \mathrm{d}x_1 \, T(x_3|x_1;\tau) \mathcal{P}_1\left(x_1, t_1\right)$$

Master equation approach IV

one has

$$\partial_\tau \mathcal{P}_1(x_3, t_1+\tau) = \int \mathrm{d}x_2 \left(W(x_3|x_2)\mathcal{P}_1(x_2, t_1+\tau) - W(x_2|x_3)\mathcal{P}_1(x_3, t_1+\tau) \right) .$$

Note: This suggests "Later PDF from earlier ones." But a master equation is about transition probabilities, applying to *every* initial state. Discrete states n:

$$\partial_t \mathcal{P}_n(t) = \sum_{n'} W(n|n')\mathcal{P}_{n'}(t) - W(n'|n)$$

A gain/loss equation.

Master equation approach V

Introduce matrix $\mathbb{W}$:

$$\mathbb{W}_{nn'} = W(n|n') - \delta_{nn'} \sum_{n''} W(n''|n)$$

(note the negative loss and positive gain) so that

$$\partial_t \mathbf{p}(t) = \mathbb{W}_{nn'} \mathbf{p}(t)$$

with formal solution $\mathbf{p}(t) = \exp\left(t\mathbb{W}_{nn'}\right)\mathbf{p}(0)$ (which may or may not exist).

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FOKKER-PLANCK equation I

One particularly important (type of) master equation is the **FOKKER-PLANCK equation.**
Write the transition rate function $W(x'|x)$ as $w(x,-r)$.

$$\begin{aligned}\partial_\tau \mathcal{P}_1(x_3,\tau) &= \int \mathrm{d}x_2\ \left(w(x_2,x_3-x_2)\mathcal{P}_1(x_2,\tau) - w(x_3,x_2-x_3)\mathcal{P}_1(x_3,\tau)\right)\\ &= \int \mathrm{d}r\ \left(w(x_3-r,r)\mathcal{P}_1(x_3-r,\tau) - w(x_3,-r)\mathcal{P}_1(x_3,\tau)\right)\end{aligned}$$

where $r = x_3 - x_2$.

FOKKER-PLANCK equation II

Expand for small r.

$$w(x_3 - r, r)\mathcal{P}_1(x_3 - r, \tau) = w(x_3, r)\mathcal{P}_1(x_3, \tau) - r\partial_x\left(w(x_3, r)\mathcal{P}_1(x_3, \tau)\right) + \frac{1}{2}r^2\partial_x^2\left(w(x_3, r)\mathcal{P}_1(x_3, \tau)\right) + \mathcal{O}(r^3)$$

…and use in the master equation:

$$\partial_\tau\mathcal{P}_1(x_3, \tau) = \int \mathrm{d}r\, \Big(w(x_3, r)\mathcal{P}_1(x_3, \tau) - r\partial_x\left(w(x_3, r)\mathcal{P}_1(x_3, \tau)\right) + \frac{1}{2}r^2\partial_x^2\left(w(x_3, r)\mathcal{P}_1(x_3, \tau)\right) - w(x_3, -r)\mathcal{P}_1(x_3, \tau)\Big)$$

FOKKER-PLANCK equation III

First and last term cancel on the right hand side. $\mathcal{P}_1(x_3, \tau)$ can be taken outside the integrals.
Define

$$\begin{aligned} A(x) &= \int \mathrm{d}r\, r w(x, r) \\ B(x) &= \int \mathrm{d}r\, r^2 w(x, r) \end{aligned}$$

so that

$$\partial_\tau \mathcal{P}_1(x, \tau) = -\partial_x \left(A(x) \mathcal{P}_1(x, \tau) \right) + \frac{1}{2} \partial_x^2 \left(B(x) \mathcal{P}_1(x, \tau) \right) \quad ,$$

FOKKER-PLANCK equation IV

Time evolution of mean:

$$\partial_t \langle x \rangle = \partial_\tau \int \mathrm{d}x\, x \mathcal{P}_1(x, \tau)$$
$$= -\int \mathrm{d}x\, x \partial_x \left(A(x)\mathcal{P}_1(x,\tau)\right) + \frac{1}{2}\int \mathrm{d}x\, x \partial_x^2 \left(B(x)\mathcal{P}_1(x,\tau)\right)$$

Dropping surface terms in an integration by parts:

$$\partial_t \langle x \rangle = \langle A(x) \rangle$$

Note: Expansion to second order is all that is needed!

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   - ORNSTEIN-UHLENBECK process
5. Critical dynamics

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LANGEVIN equations I

LANGEVIN equations are a type of stochastic (partial) differential equation.
They describe the (stochastic) time evolution of an observable (like the Heisenberg picture) as opposed to its PDF (as in the Schrödinger picture).
Note: LANGEVIN equations not universally liked by mathematicians (noise not being a function + Itō/Stratonovich dilemma)

Random walk — BROWNian motion I

Equation of motion:

$$\dot{x}(t) = \eta(t)$$

where $\eta(t)$ is white noise:

$$\left\langle \eta(t)\eta(t') \right\rangle = 2\Gamma^2 \delta(t - t') \ .$$

This noise is GAUSSian, has vanishing mean and a δ correlator, so constant spectrum. The variance is infinite.
Any integral over η is like a sum of infinitely many random variables, GAUSSian because of the CLT (central limit theorem).
Good choice:

$$\mathcal{P}\left([\eta(t)]\right) \propto e^{-\frac{1}{4\Gamma^2}\int \mathrm{d}t\, \eta(t)^2}$$

Random walk — BROWNian motion II

(probability dependent on square displacement).
Integrate equation of motion:

$$x(t) = x_0 + \int_{t_0}^{t} \mathrm{d}t' \, \eta(t') \ .$$

Take averages:

$$\langle x(t) \rangle = \langle x_0 \rangle + \left\langle \int_{t_0}^{t} \mathrm{d}t' \, \eta(t') \right\rangle = x_0$$

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Random walk — BROWNian motion III

and

$$\begin{aligned}\langle x(t_1)x(t_2)\rangle &= x_0^2 + \left\langle \int_{t_0}^{t_1} \mathrm{d}t_1' \int_{t_0}^{t_2} \mathrm{d}t_2' \, \eta(t_1')\eta(t_2') \right\rangle \\ &= x_0^2 + \int_{t_0}^{t_1} \mathrm{d}t_1' \int_{t_0}^{t_2} \mathrm{d}t_2' \, \langle \eta(t_1')\eta(t_2') \rangle = x_0^2 + \int_{t_0}^{t_1} \mathrm{d}t_1' \int_{t_0}^{t_2} \mathrm{d}t_2' \, 2\Gamma^2 \delta(t_1' - t_2')\end{aligned}$$

What is that integral? Specify $t_2 \geqslant t_1$ without loss of generality. Integral over t_2' contributes for all t_1':

$$\langle x(t_1)x(t_2)\rangle = x_0^2 + 2\Gamma^2 \min(t_1, t_2)$$

Random walk — BROWNian motion IV

General two time correlator:

$$\begin{aligned} \langle x(t_1)x(t_2)\rangle - \langle x(t_1)\rangle \langle x(t_2)\rangle \\ = \langle (x(t_1) - \langle x(t_1)\rangle)(x(t_2) - \langle x(t_2)\rangle)\rangle \\ = \langle x(t_1)x(t_2)\rangle_c \end{aligned}$$

Equal time correlator, $t_1 = t_2$, linear in t:

$$\left\langle x(t)^2 \right\rangle_c = 2\Gamma^2 t \ .$$

All higher cumulants of η vanish and so do those of $x(t)$.

ORNSTEIN-UHLENBECK process I

ORNSTEIN-UHLENBECK process

The ORNSTEIN-UHLENBECK (O-U) process is the only MARKOVian, stationary and GAUSSian process (by DOBB's theorem). It's equation of motion is

$$\dot{x}(t) = \eta(t) - \gamma x(t)$$

Note the spring-like term $-\gamma x(t)$ with spring constant γ.
Mean position $\langle \dot{x} \rangle(t) = -\gamma \langle x \rangle (t)$, so

$$\langle x(t) \rangle (x_0) = x_0 e^{-\gamma t}$$

with x_0 the starting point. At stationarity (strictly part of O-U):

$$\mathcal{P}_{\mathrm{OU}}(x_0) = \sqrt{\frac{\gamma}{2\pi\Gamma^2}} e^{-\frac{x_0^2 \gamma}{2\Gamma^2}}$$

ORNSTEIN-UHLENBECK process II

Formal solution of O-U:

$$x(t;x_0) = x_0 e^{-\gamma t} + \int_0^t \mathrm{d}t'\, \eta(t') e^{-\gamma(t-t')}$$

Two point correlation function:

$$\langle x(t_1)x(t_2)\rangle(x_0) = x_0^2 e^{-\gamma(t_1+t_2)} + 2\Gamma^2 \int_0^{t_1} \mathrm{d}t_1' \int_0^{t_2} \mathrm{d}t_2'\, \delta(t_1'-t_2') e^{-\gamma((t_1+t_2)-(t_1'+t_2'))}$$

where the first term is $x_0^2 \exp(-\gamma(t_1+t_2)) = \langle x(t_1)\rangle(x_0)\,\langle x(t_2)\rangle(x_0)$.

ORNSTEIN-UHLENBECK process III

Choose $t_2 \geqslant t_1$:

$$\langle x(t_1)x(t_2)\rangle (x_0) = x_0^2 e^{-\gamma(t_1+t_2)} + \frac{\Gamma^2}{\gamma}\left(e^{-\gamma(t_2-t_1)} - e^{-\gamma(t_2+t_1)}\right)$$

so that

$$\langle x(t_1)x(t_2)\rangle_c (x_0) = \langle x(t_1)x(t_2)\rangle (x_0) - \langle x(t_1)\rangle (x_0) \langle x(t_2)\rangle (x_0)$$
$$= \frac{\Gamma^2}{\gamma}\left(e^{-\gamma(t_2-t_1)} - e^{-\gamma(t_2+t_1)}\right)$$

Evaluate for equal times:

$$\langle x(t)x(t)\rangle_c (x_0) = \frac{\Gamma^2}{\gamma}\left(1 - e^{-2\gamma t}\right)$$

ORNSTEIN-UHLENBECK process IV

Recover BROWNian motion in the limit $\gamma \to 0$.
To find the full ORNSTEIN-UHLENBECK process (including the averaging over x_0):

$$\langle x(t_1)x(t_2)\rangle_c = \langle x(t_1)x(t_2)\rangle - \langle x\rangle(t_1)\langle x\rangle(t_1)$$

$$= \int \mathrm{d}x_0\, \mathcal{P}_{\mathsf{OU}}(x_0) \left\{ x_0^2 e^{-\gamma(t_1+t_2)} + \frac{\Gamma^2}{\gamma}\left(e^{-\gamma(t_2-t_1)} - e^{-\gamma(t_2+t_1)}\right)\right\}$$

$$= \frac{\Gamma^2}{\gamma} e^{-\gamma(t_2-t_1)}$$

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Outline

3 Random walks

4 LANGEVIN equations

5 Critical dynamics
- From HAMILTONian to LANGEVIN equation and back
- The PDF of η
- A FOKKER-PLANCK equation approach
- The HOHENBERG-HALPERIN models

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Critical dynamics I

In critical systems, time can be regarded as "just another relevant field". The free energy follows

$$f(\tau, h, t) = \lambda^{-d} f(\tau\lambda^{y_t}, h\lambda^{y_h}, t\lambda^{-z})$$

so that, for example,

$$m(0, 0, t) = \lambda^{y_h - d} m(0, 0, t\lambda^{-z})$$

and therefore

$$m(0, 0, t) = t^{-\frac{\beta}{\nu z}} m(0, 0, 1)$$

In the following: Relation between HAMILTONian and LANGEVIN, followed by brief overview.

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From HAMILTONian to LANGEVIN equation and back I

Consider the HAMILTONian of

ϕ^4 theory

$$\mathcal{H}[\phi] = \int \mathrm{d}^d x \, \frac{1}{2} (\nabla \phi)^2 + \frac{1}{2} r \phi^2 + \frac{u}{4!} \phi^4 + h(x) \phi(\mathbf{x})$$

a functional of the order parameter field $\phi(\mathbf{x})$.

Naïve relaxational dynamics minimises HAMILTONian:

$$\dot{\phi} = -D \frac{\delta \mathcal{H}}{\delta \phi}$$

so in ϕ^4:

$$\dot{\phi} = D(\nabla^2 \phi - r\phi + \frac{u}{6} \phi^3 + h)$$

From HAMILTONian to LANGEVIN equation and back II

Add noise for fluctuations — in total:

$$\dot{\phi}(\mathbf{x},t) = D\left(\nabla^2\phi(\mathbf{x},t) - r\phi(\mathbf{x},t) + \frac{u}{6}\phi(\mathbf{x},t)^3 + h(\mathbf{x},t)\right) + \eta(\mathbf{x},t)$$

known as **model A** or GLAUBER dynamics. The noise correlator is

$$\left\langle\eta(\mathbf{x},t)\eta(\mathbf{x}',t')\right\rangle = 2\Gamma^2\delta(t-t')\delta(\mathbf{x}-\mathbf{x}')\ .$$

General form:

$$\dot{\phi}(\mathbf{x},t) = -D\left.\frac{\delta\mathcal{H}([\psi])}{\delta\psi(\mathbf{x})}\right|_{\phi(\mathbf{x})=\phi(\mathbf{x},t)} + \eta(\mathbf{x},t)$$

Note that the HAMILTONian is not differentiated with respect to a time dependent function.

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The PDF of η I

The following tries to develop an understanding of the noise, for the time being a function only of time t (not of space $\mathbf{x}$).

Consider discrete random variables η_i with variance

$$\langle \eta_i \eta_j \rangle = 2\Gamma^2 \delta_{ij} \Delta t^{-1}$$

and vanishing mean. Their distribution is a GAUSSian:

$$\mathcal{P}_i(\eta) = \sqrt{\frac{\Delta t}{4\pi\Gamma^2}} e^{-\frac{\eta^2 \Delta t}{4\Gamma^2}}$$

The joint distribution of the independent random variables is

$$\mathcal{P}(\eta_1, \ldots, \eta_n) = \left(\frac{\Delta t}{4\pi\Gamma^2}\right)^{n/2} e^{-\frac{\Delta t \sum_i^n \eta_i^2}{4\Gamma^2}}$$

The PDF of η II

and in the continuum limit (without normalisation):

$$\mathcal{P}\left([\eta(t)]\right) \propto e^{-\frac{1}{4\Gamma^2}\int \mathrm{d}t\, \eta(t)^2} .$$

An average is written

$$\langle \bullet \rangle = \int \mathcal{D}\eta \mathcal{P}\left([\eta(t)]\right) \bullet$$

where $\mathcal{D}\eta$ stands for $\prod \mathrm{d}\eta_i$ if time is discretised again.
The moment generating function of the noise is $\left\langle \exp\left(\int \mathrm{d}t\, \eta h(t)\right)\right\rangle$ with $h(t)$ a function of time. Completing the squares

$$-\frac{1}{4\Gamma^2}\eta(t)^2 + \eta(t)h(t) = -\frac{1}{4\Gamma^2}\left(\eta(t) - 2\Gamma^2 h(t)\right)^2 + \Gamma^2 h(t)^2$$

The PDF of η III

allows us to perform the GAUSSian integrals, so that

$$\left\langle e^{\int \mathrm{d}t\, \eta h(t)} \right\rangle = e^{\int \mathrm{d}t\, \Gamma^2 h(t)^2}$$

Differentiating functionally twice with respect to $h(t)$ gives the correlator

$$\frac{\delta^2}{\delta h(t) \delta h(t')} \ln \left\langle e^{\int \mathrm{d}t\, \eta h(t)} \right\rangle = \frac{\delta^2}{\delta h(t) \delta h(t')} \int \mathrm{d}t\, \Gamma^2 h(t)^2 = 2\Gamma^2 \delta(t - t')$$

reproducing the correlator for η introduced above.
Generalise for space dependence:

$$\mathcal{P}\left([\eta(\mathbf{x}, t)]\right) \propto e^{-\frac{1}{4\Gamma^2} \int \mathrm{d}t \mathrm{d}^d x\, \eta(\mathbf{x},t)^2}$$

The PDF of η IV

Consider a LANGEVIN equation of the form

$$\partial_t \phi(\mathbf{x}, t) = -\mathcal{F}[\phi] + \eta(\mathbf{x}, t)$$

An observable $\bullet$ which is a function of a solution $\phi(\mathbf{x}, t)$ has expectation value

$$\langle \bullet \rangle = \int \mathcal{D}\phi \exp\left(-\frac{1}{4\Gamma^2} \int \mathrm{d}t \mathrm{d}^d x \, [\partial_t \phi(\mathbf{x}, t) - \mathcal{F}[\phi]]^2 \right)$$

where $\eta = \partial_t \phi + \mathcal{F}[\phi]$ was used and the integration measure $\mathcal{D}\eta$ was replaced by $\mathcal{D}\phi$ with a JACOBian that turns out to be unity. With

$$-\mathcal{F}[\phi(\mathbf{x}, t)] = D \frac{\delta \mathcal{H}([\psi])}{\delta \psi(\mathbf{x})} \bigg|_{\phi(\mathbf{x}) = \phi(\mathbf{x}, t)} =: D\mathcal{H}'([\phi(\mathbf{x}, t)])$$

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The PDF of η V

one arrives at the ONSAGER-MACHLUP functional

$$\langle \bullet \rangle = \int \mathcal{D}\phi \exp\left(-\frac{1}{4\Gamma^2} \int \mathrm{d}t' \mathrm{d}^d x' \, \left[\partial_t \phi(\mathbf{x}', t') + D\mathcal{H}'([\phi(\mathbf{x}', t')]) \right]^2 \right) \bullet$$

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A FOKKER-PLANCK equation approach I

From the LANGEVIN equation derived above, a FOKKER-PLANCK equation can be derived (following Zinn-Justin, 1997). For the time being, the field ϕ is only time-dependent.
Consider

$$\dot{\phi}(t) = -D\, \partial_\psi\big|_{\phi(t)} \mathcal{H}(\psi) + \eta(t)$$

Simplify notation: $\partial_\psi\big|_{\phi(t)} \mathcal{H}(\psi) = \mathcal{H}'(\phi)$
The probability of ϕ to have value ϕ_0 at time t is

$$\mathcal{P}_\phi\left(\phi_0; t\right) = \langle \delta(\phi(t) - \phi_0) \rangle$$

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A FOKKER-PLANCK equation approach II

The time evolution follows:

$$\begin{aligned}\partial_t \mathcal{P}_\phi(\phi_0;t) &= \partial_t \langle \delta(\phi(t)-\phi_0)\rangle \\ &= \left\langle \dot{\phi}(t)\frac{\partial}{\partial\phi}\delta(\phi(t)-\phi_0)\right\rangle\end{aligned}$$

In the following, when taking averages $\langle\bullet\rangle$, the field ϕ is to be interpreted a functional of η (the convolution of η with the propagator), or η is to be interpreted a new dummy variable depending on ϕ.
Next: $\partial_\phi\delta(\phi-\phi_0) = -\partial_{\phi_0}\delta(\phi-\phi_0)$, so that

$$\partial_t \mathcal{P}_\phi(\phi_0;t) = -\partial_{\phi_0}\left\langle\left(-D\mathcal{H}'(\phi(t))+\eta(t)\right)\delta(\phi(t)-\phi_0)\right\rangle$$

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A FOKKER-PLANCK equation approach III

The first term is found

$$\left\langle -D\mathcal{H}'(\phi(t))\delta(\phi(t)-\phi_0)\right\rangle = -D\mathcal{H}'(\phi_0)\left\langle\delta(\phi(t)-\phi_0)\right\rangle = -D\mathcal{H}'(\phi_0)\mathcal{P}_\phi(\phi_0;t) \ .$$

the second term is more difficult, $\langle\eta(t)\delta(\phi(t)-\phi_0)\rangle$.
Note:

$$\int\mathcal{D}\eta\frac{\delta}{\delta\eta(t)}\exp\left(-\frac{1}{4\Gamma^2}\int dt'\,\eta(t')^2\right) = \int\mathcal{D}\eta\left(-\frac{1}{2\Gamma^2}\eta(t)\right)\exp\left(-\frac{1}{4\Gamma^2}\int dt'\,\eta(t')^2\right)$$

A FOKKER-PLANCK equation approach IV

and by functional integration by parts (see Zinn-Justin, 1997)

$$
\begin{aligned}
&\langle \eta(t)\delta(\phi(t)-\phi_0)\rangle \\
&\quad = -2\Gamma^2 \int \mathcal{D}\eta\, \delta(\phi(t)-\phi_0) \frac{\delta}{\delta\eta(t)} \exp\left(-\frac{1}{4\Gamma^2}\int \mathrm{d}t'\, \eta(t')^2\right) \\
&\quad = 2\Gamma^2 \int \mathcal{D}\eta \exp\left(-\frac{1}{4\Gamma^2}\int \mathrm{d}t'\, \eta(t')^2\right) \frac{\delta}{\delta\eta(t)} \delta(\phi(t)-\phi_0) \\
&\quad = 2\Gamma^2 \left\langle \frac{\delta}{\delta\eta(t)} \delta(\phi(t)-\phi_0) \right\rangle
\end{aligned}
$$

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A FOKKER-PLANCK equation approach V

$\phi(t)$ is a functional of η, as a matter of choice (Itô/Stratonovich dilemma)

$$\frac{\delta}{\delta\eta(t)}\phi(t) = \frac{1}{2}$$

so that

$$\left\langle \frac{\delta}{\delta\eta(t)}\delta(\phi(t)-\phi_0) \right\rangle = \frac{1}{2}\partial_{\phi(t)} \langle\delta(\phi(t)-\phi_0)\rangle$$
$$= -\frac{1}{2}\partial_{\phi_0} \langle\delta(\phi(t)-\phi_0)\rangle$$
$$= -\frac{1}{2}\partial_{\phi_0}\mathcal{P}_{\phi}(\phi_0;t)$$

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A FOKKER-PLANCK equation approach VI

Collecting terms, the FOKKER-PLANCK equation is found:

$$\partial_t \mathcal{P}_\phi(\phi_0;t) = \partial_{\phi_0}\left(D\mathcal{H}'(\phi_0)\mathcal{P}_\phi(\phi_0;t)\right) + \Gamma^2\partial^2_{\phi_0}\mathcal{P}_\phi(\phi_0;t) \quad .$$

At stationarity $\partial_t \mathcal{P}_\phi(\phi_0;t) = 0$ and therefore

$$\partial_{\phi_0}\left(D\mathcal{H}'(\phi_0)\mathcal{P}_\phi(\phi_0;t) + \Gamma^2\partial_{\phi_0}\mathcal{P}_\phi(\phi_0;t)\right) = 0$$

one solution is the MAXWELL-BOLTZMANN distribution:

$$\mathcal{P}_{\phi;\mathrm{stat}}(\phi) \propto e^{-\frac{D}{\Gamma^2}\mathcal{H}([\phi])} \quad ,$$

easily extended to space dependent HAMILTONians.

The HOHENBERG-HALPERIN models

- Time-evolution of statistical systems, in particular response to perturbation, is the subject of non-equilibrium statistical mechanics.
- LANGEVIN equations derived from a HAMILTONian and producing MAXWELL-BOLTZMANN are known as **non-equilibrium models relaxing to equilibrium.**
- LANGEVIN equations which are not based on a HAMILTONian are generally said to be **far-from-equilibrium models.**
- Sometimes the former is referred to **equilibrium dynamics**, the latter as **non-equilibrium dynamics**.

The HOHENBERG-HALPERIN models

Standard models relaxing to equilibrium

Model A, GLAUBER dynamics

$$\dot{\phi}(\mathbf{x},t) = D\left(\nabla^2\phi(\mathbf{x},t) - r\phi(\mathbf{x},t) + \frac{u}{6}\phi(\mathbf{x},t)^3 + h(\mathbf{x},t)\right) + \eta(\mathbf{x},t) \ ,$$

The most basic dynamics of ϕ^4 theory.

The HOHENBERG-HALPERIN models

Standard models relaxing to equilibrium

Model B, KAWASAKI dynamics

$$\dot{\phi}(\mathbf{x},t) = -\nabla^2 D\left(\nabla^2\phi(\mathbf{x},t) - r\phi(\mathbf{x},t) + \frac{u}{6}\phi(\mathbf{x},t)^3 + h(\mathbf{x},t)\right) + \zeta(\mathbf{x},t)$$

with noise $\zeta = \nabla\eta$, so that the right hand side is a gradient.
This model has **conserved order parameter.**

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The HOHENBERG-HALPERIN models

Standard models relaxing to equilibrium

Models C, D, J, E, G

- Model C: Conserved energy density ρ with non-conserved order parameter
- Model D: Conserved energy density ρ with conserved order parameter
- Model J: Non-scalar order parameter
- Model E: Anisotropy
- Model G: Anisotropy and anti-ferromagnetic coupling constant

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Enjoy!