Analysis of Reaction-Diffusion Processes by Field Theoretic Methods

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Outline

Introduction

- What does field theory “normally” look like?
- Advantages and disadvantages?
- Field theory for reaction diffusion processes.

ϕ^4 theory

Basic ingredients of a field theory

- Continuous, local degrees of freedom $\phi(\mathbf{x})$.
- Parameterisation by a few couplings, say r, u.
- Build Hamiltonian (energy), motivated by some effective theory, by symmetries, mean field ideas, lowest order expansions *etc.*, say

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

- Use Hamiltonian in Boltzmann factor, exp $\left(-\mathcal{H}/(k_b T)\right)$.
- Add external (source) field $j(\mathbf{x})$ for generating moments.

Absorb $k_b T$ and write path integral:

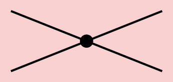
$$\mathcal{Z}[j] = \int \mathcal{D}\phi \, \exp\left(-\int \mathrm{d}^d x \, \frac{1}{2} r \phi^2(\mathbf{x}) + \frac{1}{2} \left(\nabla\phi(\mathbf{x})\right)^2 + \frac{u}{4!}\phi^4(\mathbf{x}) - j(\mathbf{x})\phi(\mathbf{x})\right)$$

ϕ^4 theory I

Diagrams

Perturbative expansion of the partition sum:

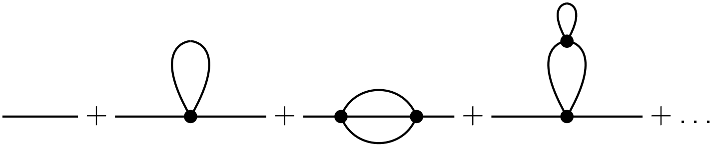
$$\mathcal{Z}[j] = \int \mathcal{D}\phi \, \exp\left(- \int \mathrm{d}^d x \; \frac{1}{2} r \phi^2(\mathbf{x}) + \frac{1}{2} \left(\nabla\phi(\mathbf{x})\right)^2 + \frac{u}{4!}\phi^4(\mathbf{x}) - j(\mathbf{x})\phi(\mathbf{x}) \right)$$



ϕ^4 theory II

Diagrams

Expand diagramatically for small u, for example:

$\langle \phi\phi \rangle_c =$ 

- *Effective* Hamiltonian (right symmetries etc).
- *Exact* partition sum.
- *Perturbative* treatment of interaction.
- Physics of diagrams?
- Special attention needed for infinities (characterise long range behaviour).

ϕ^4 theory

The bare propagator

$$\langle \phi\phi \rangle_{c,0} = \text{———} = \frac{1}{\mathbf{k}^2 + r}$$

In real space:

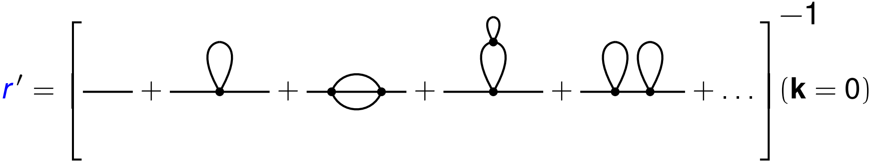
$$\left\langle \phi(\mathbf{x})\phi(\mathbf{x}') \right\rangle_{c,0} = |\mathbf{x} - \mathbf{x}'|^{-(d-2)} \mathcal{G}\left(|\mathbf{x} - \mathbf{x}'|\sqrt{r}\right)$$

and in $d = 1, 3$ scaling function $\mathcal{G}$ is an exponential.
The “mass” r cuts off the correlation, *i.e.* it provides a characteristic length, $\xi = 1/\sqrt{r}$.

ϕ^4 theory

The meaning of mass r

Renormalised mass (inverse full propagator at $\mathbf{k} = 0$)



to be used in a simplified theory (using only the simplest diagrams), incorporating *some* of the effect of the interaction.

Here: Interaction reduces correlation length (increases mass).

Very useful — But where is the physics?

Non-equilibrium field theories

- Extension to non-equilibrium "straight forward" (Martin, Siggia, Rose, Janssen, De-Dominicis).
- Boltzmann factor $\exp\left(-\mathcal{H}/(k_b T)\right)$ turns into integrand giving rise to a δ-function.
- Effective action replaces Hamiltonian.

Why is this method not widely used in complexity?

- Requires Langevin or Fokker-Planck equation as starting point.
- Focus on long range, long time (which might still be very helpful).
- Focus on asymptotes (which might not be so helpful).
- Effective theories in, effective theories out. Physics gone!

The Answer: Second Quantisation

Use the language of
second quantisati$o^\dagger\,|n\rangle$
to describe complex
systems!

Key features

- Scheme goes back to Doi (1976) and Peliti (1985).
- Use creation and annihilation operators to represent particle interaction in master equation.
- Field theory arises as a Legendre transform of the time evolution operator (Liouvillian).
- Degrees of freedom remain discrete, even space can remain discrete.
- Diagrammatic expansion, couplings etc. retain physics (not an *effective* theory).

Creation and Annihilation Operators

J Cardy, *Lecture notes*, 1998, 2006

The key ingredient in the construction of the field theory are the creation and annihilation (ladder) operators that differ only slightly from those "normally" used in Quantum Mechanics:

$$\begin{aligned} a^\dagger(\mathbf{x})\,|n_\mathbf{x}\rangle &= |n_\mathbf{x}+1\rangle \\ a(\mathbf{x})\,|n_\mathbf{x}\rangle &= n_\mathbf{x}\,|n_\mathbf{x}-1\rangle \end{aligned}$$

$|n_\mathbf{x}\rangle$ is a configuration with $n_\mathbf{x}$ at site $\mathbf{x}$. These "coherent states" are eigenstates of the particle number operator

$$a^\dagger(\mathbf{x})a(\mathbf{x})\,|n_\mathbf{x}\rangle = n_\mathbf{x}\,|n_\mathbf{x}\rangle$$

$|0\rangle$ is the empty system.

From master equation to creation/annihilation I

J Cardy, *Lecture notes*, 1998, 2006

Particles hoping with rate D from 1 to 2:

$$\frac{\mathrm{d}}{\mathrm{d}t}P(n_1, n_2; t) = D(n_1+1)P(n_1+1, n_2-1) - Dn_1 P(n_1, n_2)$$

The "average configuration" is

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

From master equation to creation/annihilation II

J Cardy, *Lecture notes*, 1998, 2006

How does $|\psi\rangle(t)$ evolve in time? Differentiate and note:

$$\sum_{n_1,n_2} D(n_1+1)P(n_1+1,n_2-1){a_1^\dagger}^{n_1}{a_2^\dagger}^{n_2}|0\rangle$$
$$= \sum_{n_1,n_2} DP(n_1+1,n_2-1)a_2^\dagger a_1 {a_1^\dagger}^{n_1+1}{a_2^\dagger}^{n_2-1}|0\rangle$$
$$= a_2^\dagger a_1 \sum_{n_1,n_2} DP(n_1,n_2){a_1^\dagger}^{n_1}{a_2^\dagger}^{n_2}|0\rangle$$

using $P(n_1,-1)=0$ (no negative occupation) and $a_1{a_2^\dagger}^{n_2}|0\rangle = 0$ (no annihilation at 1 if no particle at 1).
The hopping from 1 to 2 thus becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}|\psi\rangle(t) = D\left(a_2^\dagger a_1 - a_1^\dagger a_1\right)|\psi\rangle(t)$$

From master equation to creation/annihilation III

J Cardy, *Lecture notes*, 1998, 2006

Extension to random walk straight forward

$$\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi\right\rangle(t) = -\frac{1}{2}D\sum_{\mathbf{n}}\sum_{\mathbf{m}\text{ nn of }\mathbf{n}}\left(a^\dagger(\mathbf{n}) - a^\dagger(\mathbf{m})\right)\left(a(\mathbf{n}) - a(\mathbf{m})\right)\left|\psi\right\rangle(t)$$

Sum double counts nearest neighbour pairs.
Formal solution:

$$\left|\psi\right\rangle(t) = e^{-\mathcal{L}t}\left|\psi\right\rangle(0)$$

with

$$\mathcal{L} = \frac{1}{2}D\sum_{\mathbf{n}}\sum_{\mathbf{m}\text{ nn of }\mathbf{n}}\left(a^\dagger(\mathbf{n}) - a^\dagger(\mathbf{m})\right)\left(a(\mathbf{n}) - a(\mathbf{m})\right) + \ldots$$

Another example follows.

A path integral representation

Path integral generated by considering time discretisation:

$$e^{-\mathcal{L}t} = \lim_{\Delta t \to 0} (1 - \mathcal{L}t)^{t/\Delta t}$$

and the Laplace transform

$$(2\pi)^{-1} \int \mathrm{d}\phi^* \wedge \mathrm{d}\phi \, e^{-\phi^*\phi} e^{\phi a^\dagger} |0\rangle \langle 0| e^{\phi^* a} = \sum_n \left(a^\dagger\right)^n |0\rangle \langle 0| \frac{a^n}{n!} = 1$$

which allows us (after some tricks, such as the Doi shift $\phi^* \to 1 + \phi^*$) to write the generating functional as a path integral:

$$\mathcal{Z}[j^\dagger, j] = \langle 0| \exp\left(-\int \mathrm{d}t \, \mathcal{L}[a^\dagger, a] - \int \mathrm{d}^d x \, j a(\mathbf{x}) - j^\dagger a^\dagger(\mathbf{x})\right) |0\rangle$$

$$= \int \mathcal{D}\phi^\dagger \, \mathcal{D}\phi \, \exp\left(-\int \mathrm{d}t \, \mathcal{L}[\phi^\dagger(\mathbf{x}, t), \phi(\mathbf{x}, t)] - \int \mathrm{d}^d x \, j\phi(\mathbf{x}, t) - j^\dagger \phi^*(\mathbf{x}, t)\right)$$

At this stage, the field theory in the continuous degree of freedom ϕ is still exact, even when the original degree of freedom is discrete. Even space and time can still be be chosen to be discrete.

Building a field theory

The Gaussian part of the field theory can be integrated:

$$\mathcal{Z}_0 = \int \mathcal{D}\phi^\dagger \mathcal{D}\phi \; \exp\left(- \int \mathrm{d}t\mathrm{d}^d x \; \phi^\dagger \partial_t \phi + D \nabla\phi^\dagger \nabla\phi + \int \mathrm{d}^d x \; ja + j^\dagger a^\dagger \right)$$

gives in **k**-space:

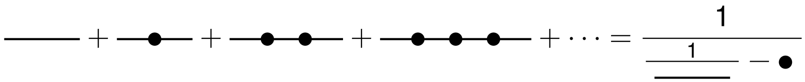
$$\mathcal{Z}_0 = \exp\left(\int đ\omega \, đ^d k \, j^\dagger(\mathbf{k}, \omega)(-\imath\omega + D\mathbf{k}^2)^{-1} j(\mathbf{k}, \omega) \right)$$

and so the connected correlation function is

$$\langle \phi\phi \rangle_{c,0} = \rule{2cm}{0.4pt} = \frac{1}{-\imath\omega + D\mathbf{k}^2}$$

Perturbation Theory

Analysis of non-(bi)linearities proceeds perturbatively in the Gaussian theory.
Integrals are written in diagrams.
Loops and multiple interactions can be (re)summed into effective couplings:



Large scale, long time behaviour if necessary determined by renormalised field theory, using spurious ultraviolet divergences to characterise the infrared.

Outline

Pros and cons of the field theoretic description

- Degrees of freedom remain discrete.
- Procedure of writing the path integral *generates* effective processes.
- Diagrams reflect the physics of the process.
- Scheme easily extended to general graphs.
- Spatial continuum not necessary.
- Boundaries can be dealt with.
- Results are easily derived . . . after significant preparatory work.
- Might require numerical evaluation of sums.
- Irrelevant terms should be dropped for simplicity, but might contain interesting physics.
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Summary

- Traditional field theoretic methods are powerful but hide the physics.
- Continuum description (degree of freedom and/or space and/or time) often inadequate.
- Second quantisation (Doi, Pelitti, reaction-diffusion) generates physically tractable field theory.
- Provides insight into effective processes and easy access to relevant observables.
- Use it for diffusion, branching, voting *etc.* on regular lattices and general graphs.

Thank you!