A field theoretic approach to the Wiener Sausage

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Outline

- Field theoretic approach to emergent phenomena
- 2 Application: The Wiener Sausage

3 Field Theory

- 4 Renormalisation
- 5 Results on regular lattices

Field theoretic approach to emergent phenomena

Field Theory:

- Fields are continuous degrees of freedom normally defined at every point in space and time.
- Equation of motion of fields (*e.g.* Maxwell equations).
- Description of choice for **cooperative phenomena**.
- Often: Focus on long range, long time (which might still be very helpful).
- Focus on exponents of asymptotes (which might not be so helpful).
- Often: Effective theories in, effective theories out. Physics gone !?

Second Quantisation

Idea: Use language of Quantum Field Theory to describe reaction-diffusion processes (*e.g.* Smoluchowski):

- Coarse grained degrees of freedom readily available.
- Particle nature retained (*e.g.* single particle diffusion).
- Poisson processes.
- Renormalisation reveals *effective* processes (*e.g.* diffusion via proliferation).

Specifically: Doi-Peliti.

Key features of Doi-Peliti

- 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).
- Physical degrees of freedom remain discrete, fields as conjugate variables in generating functions.
- Space can remain discrete.
- Diagrammatic expansion, couplings etc. retain physics (not an *effective* theory).
- No need to throw away irrelevant terms; many features away from the critical point remain accessible (not part of this talk).

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:

$$\begin{array}{rcl} a^{\dagger}(\mathbf{x}) \left| n_{\mathbf{x}} \right\rangle & = & \left| n_{\mathbf{x}} + 1 \right\rangle \\ a(\mathbf{x}) \left| n_{\mathbf{x}} \right\rangle & = & n_{\mathbf{x}} \left| n_{\mathbf{x}} - 1 \right\rangle \end{array}$$

 $|n_x\rangle$ is a configuration with n_x particles at site x. These "pure 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 hopping with rate *D* from 1 to 2:

 $\frac{\mathrm{d}}{\mathrm{d}t}P(n_1, n_2; t) = D(n_1 + 1)P(n_1 + 1, n_2 - 1) - Dn_1P(n_1, n_2)$

The "generating function" 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:

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

= $\sum_{n_1,n_2} DP(n_1+1,n_2-1)a_2^{\dagger}a_1a_1^{\dagger n_1+1}a_2^{\dagger n_2-1} |0\rangle$
= $a_2^{\dagger}a_1\sum_{n_1,n_2} DP(n_1,n_2)a_1^{\dagger n_1}a_2^{\dagger n_2} |0\rangle$

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

From master equation to creation/annihilation III J Cardy, *Lecture notes*, 1998, 2006

Extension to random walk straight forward

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

Sum double counts nearest neighbour pairs. Formal solution:

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

with

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

Another example follows.

A path integral representation

Path integral generated by considering time discretisation:

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

and the Laplace transform

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

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

$$\begin{aligned} \mathcal{Z}[j^{\dagger},j] &= \langle 0| \int \mathcal{D}\phi^{\dagger} \mathcal{D}\phi \, \exp\left(-\int \mathrm{d}t \, \mathcal{L}[\phi^{\dagger}(\mathbf{x},t),\phi(\mathbf{x},t)] \right. \\ &\left. - \int \mathrm{d}^{d}x \mathrm{d}t j \phi(\mathbf{x},t) - j^{\dagger} \phi^{*}(\mathbf{x},t) - \phi^{*}(\mathbf{x},t) \partial_{t} \phi(\mathbf{x},t) \right) \end{aligned}$$

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.

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Field Theory for the Wiener

Building a field theory

The Gaussian part of the field theory can be integrated:

$$\mathcal{Z}_{0} = \int \mathcal{D}\phi^{\dagger} \mathcal{D}\phi \exp\left(-\int dt d^{d}x \,\phi^{\dagger} \partial_{t}\phi + D\nabla\phi^{\dagger}\nabla\phi + \int dt d^{d}x \,j\phi + j^{\dagger}\phi^{\dagger}\right)$$

gives in k, w-space:

$$\mathcal{Z}_{0} = \exp\left(\int \mathbf{d}\,\boldsymbol{\omega}\,\mathbf{d}^{d}k j^{\dagger}(\mathbf{k},\boldsymbol{\omega})(-\mathbf{i}\boldsymbol{\omega} + D\mathbf{k}^{2})^{-1}j(\mathbf{k},\boldsymbol{\omega})\right)$$

and so the connected correlation function is

$$\langle \phi \phi \rangle_{c,0} = ----= \frac{1}{-i\omega + D\mathbf{k}^2}$$

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.

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The other Wiener!



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Wiener process

(named after Norbert Wiener)

Consider a random walker in 2D, leaving a trace:

Think of the random walker (red dot) as the tip of a pen, spilling ink.

What is the area covered in blue (volume of a "Wiener sausage", traced out in one, two, three dimensions)?

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Motivation

- Original problem (average area, 2D) solved by Kolmogoroff and Leontowitsch (1933).
- Famously studied by Spitzer, Kac and Luttinger.
- "Wiener Sausage Volume Moments" by Berezhkovskii, Makhnovskii and Suris (1989).
- Applications ...
- Lots of variants and extensions...

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- Applications in
 - Medicine, *e.g.* tissue "priming", Dagdug, Berezhkovskii and Weiss (2002).
 - Chemical engineering, e.g. agglomerates forming by "sweeping particles", Eggersdorfer and Pratsinis (2014).
 - Ecology, *e.g.* feeding plankton, Visser (2007).
 - ▶ ...
- Lots of variants and extensions...

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- Lots of variants and extensions
 - Presence of traps, *e.g.* Oshanin, Bénichou, Coppey, and Moreau (2002).
 - Surface of the sausage, *e.g.* Rataj, Schmidt and Sporadev (2009).
 - Different boundary conditions, *e.g.* Dagdug, Berezhkovskii and Weiss (2002).
 - ▶ ...

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Determine the volume of the Wiener using Statistical Field Theory

Keeping track of a walker's trace is hard. Easy (-ier, -ish): Walker spatters ink as it walks.

Asymptotic statistics of spatter is that of a continuous trace.

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Field Theory for the Wiener

Poissonian modification

Wiener Sausage observable difficult in a field theory. Therefore:

Poissonian modification

On the lattice: With Poisson rate *H* walker jumps to a nearest neighbouring site, with rate γ attempts to place immobile offspring at current site.

Deposition suppressed if immobile particle is present already.

Anticipate regularisation: Add extinction rate ϵ' and *r* for immobile species and walkers respectively.

Mean field approach: $\partial_t \rho_s = \rho_a (1 - \rho_s) \gamma$, where ρ_s number of immobile offspring and ρ_a number density of walkers. (ρ_s is a functional of [the entire history of] ρ_a)

Perturbation theory: $\rho_a(1-\rho_s)\gamma = \gamma\rho_a - \gamma\rho_a\rho_s$.

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Perturbation theory

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Implementation of the suppressed deposition by

- (to first order) allowing unrestricted deposition
- (to second order) removing excess (deposited) particles

The suppression is difficult to deal with.

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Motivation for a field theory

Motivation for a *field theoretic* study:

- Benefit: Very flexible regarding boundary conditions, additional interactions *etc.*; Very elegant.
- Two species field theory ...
- ... with immobile particles ...
- ... and observables that are spatial integrals.
- "Doable" version of a "heavy duty" field theory.
- Guinea pig example of a fermionic problem (excluded volume constraint).

Excluded volumes are difficult in field theories. May require fermionic treatment (painful).

Idea: Introduce carrying capacity *C*, whereby deposition rate drops linearly in the occupation, $1 - \rho_s/C$. No cheating!

Using a field theory

Step by step:

- Write down master equation (maybe with carrying capacity).
- Prevision of a sector and a sector a se
- Extract propagators and vertices to create diagrams.
- Dimensional analysis, extract relevant couplings, demonstrate renormalisability.
- Calculate relevant diagrams, renormalise, extract exponents and other universal quantities.

Have fun!

Master equation: Bilinear parts — Easy



Master equation: Non-linear parts — Difficult

$$\partial_{t} \mathcal{P}(\dots, n, m, \dots) = \sum_{\mathbf{x}} \frac{\text{bilinear terms} \dots}{\left| -\gamma n \left(1 - \frac{m}{C}\right) \mathcal{P}(\dots, n, m, \dots)} \right|} + \frac{\gamma n \left(1 - \frac{m-1}{C}\right) \mathcal{P}(\dots, n, m-1, \dots)}{\text{deposition}}$$

2 Operators (Doi-Pelitti technique)

i) Introduce raising and lowering operators

$$a^{\dagger} |n\rangle = |n+1\rangle$$
 and $a |n\rangle = n |n-1\rangle$
 $b^{\dagger} |n\rangle = |n+1\rangle$ and $b |n\rangle = n |n-1\rangle$

ii) Introduce state-vector / generating function

$$|\Psi\rangle(t) = \sum_{\{n,m\}} \mathcal{P}(\ldots, n, m, \ldots) \prod_{\mathbf{x}} a^{\dagger n}(\mathbf{x}) \prod_{\mathbf{x}} b^{\dagger m}(\mathbf{x}) |0\rangle$$

Expectation $\langle \bullet \rangle = \langle \Psi_0 | \bullet | \Psi \rangle$ with suitable left vector $\langle \Psi_0 |$.

Operators (Doi-Pelitti technique)

iii) Doi-shift operators to simplify diagrammatic expansion:

$$a^{\dagger} = 1 + \tilde{a}$$
 and $b^{\dagger} = 1 + \tilde{b}$

iv) Rewrite master equation

$$\partial_t \mathcal{P}(\dots, n, m, \dots) = \sum_{\mathbf{x}} \text{ bilinear terms } \dots$$
$$-\gamma n \left(1 - \frac{m}{C}\right) \mathcal{P}(\dots, n, m, \dots) + \gamma n \left(1 - \frac{m-1}{C}\right) \mathcal{P}(\dots, n, m-1, \dots)$$

as (term-by-term, messy):

$$\partial_t |\Psi\rangle(t) = \text{bilinear terms} +$$

$$\sum_{\mathbf{x}} \gamma \tilde{b}(\mathbf{x}) a^{\dagger}(\mathbf{x}) a(\mathbf{x}) - \frac{\gamma}{C} \tilde{b}(\mathbf{r}) b^{\dagger}(\mathbf{r}) b(\mathbf{r}) a^{\dagger}(\mathbf{r}) a(\mathbf{r})$$

2 Operators (Doi-Pelitti technique)

v) Introduce Liouvillian:

$$\partial_{t} |\Psi\rangle(t) = \sum_{\mathbf{x}} \text{ bilinear terms } \dots$$

$$+\gamma \,\tilde{b}(\mathbf{x}) \,a^{\dagger}(\mathbf{x})a(\mathbf{x}) \qquad -\frac{\gamma}{C} \,\tilde{b}(\mathbf{r})b^{\dagger}(\mathbf{r})b(\mathbf{r}) \,a^{\dagger}(\mathbf{r})a(\mathbf{r})$$

$$\mathcal{L}_{1} = -\gamma \tilde{\psi} \phi^{*} \phi \qquad +\frac{\gamma}{C} \,\tilde{\psi} \psi^{*} \psi \phi^{*} \phi$$

vi) Path integral re-formulation

$$\int \mathcal{D}\tilde{\boldsymbol{\Phi}}\mathcal{D}\boldsymbol{\Phi}\mathcal{D}\tilde{\boldsymbol{\Psi}}\mathcal{D}\boldsymbol{\Psi}\exp\left(-\int d^{d}kd\,\omega\left(\mathcal{L}_{0}+\mathcal{L}_{1}\right)\right)$$



Extract bare propagators:

Allow for different renormalisation of initially identical couplings. Dimensional analysis: upper critical dimension $d_c = 2$.

Interaction vertices

Different couplings to allow different renormalisation:



Interaction vertices

Different couplings to allow different renormalisation:



Interaction vertices

Different couplings to allow different renormalisation:



Field Theory Tree level in the bulk (d > 2)

Deposition is suppressed in the presence of deposits. *Without* that, deposits could be found all along the walker's trajectory (multiple deposits at revisited sites):

This diagram is present at tree level. Although it cannot be integrated out, its contribution to correlation functions can be determined easily.

Tree level in the bulk (d > 2)

- Tree level = no loops (return asymptotically irrelevant)
- Non-linearities present at tree level.
- *n*'th moment of the sausage volume *a* dominated¹ by trees with *n* branches:

Reproduces Poissonian results above...

¹Lower order terms from other trees.

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Field Theory for the Wiener

Full theory for the bulk (d < 2)

• ... and leaves behind a trace in the form of branched-off particles:

$$\overrightarrow{}$$
 $\overleftarrow{}$ $\overleftarrow{}$ $\overleftarrow{}$ $b^{\dagger}(\mathbf{x})a^{\dagger}(\mathbf{x})a(\mathbf{x})$

• No deposition if a particle is there already:

$$\frac{}{} b^{\dagger}(\mathbf{x})b(\mathbf{x})a^{\dagger}(\mathbf{x})a(\mathbf{x})$$

• Substrate particles stuck on the lattice: -------= $\frac{1}{-i\omega + \epsilon'}$

Field Theory Meaning of vertices

This diagram probes the lattice for deposits (and suppresses further deposition):

Without it, no loops can be formed \longrightarrow tree level theory.

Interaction of the walker with its past trace.

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Calculate features of the Wiener sausage using **renormalisation**. Deposition along the trajectory

... is reduced by suppression of deposition

Loop = interaction = signature of collective phenomenon





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Calculate features of the Wiener sausage using **renormalisation**. Deposition along the trajectory

... is reduced by suppression of deposition

$$= \int \mathbf{d} \omega' \mathbf{d}' k' \frac{1}{-\mathbf{i} \omega' + D\mathbf{k}'^2} \frac{1}{\mathbf{i} \omega' + \epsilon'}$$

Physical origin of UV divergence: Time spent² per volume element diverges at $d \ge 2 = d_u$, upper critical dimension. Above: interaction irrelevant, size of sphere enters.

²Lingering, not returning, $\int dt (4Dt\pi)^{-d/2} \exp(-(x-x')^2/(4Dt))$.

Field Theory for the Wiener London

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Field Theory Benormalisation

At the heart of the theory is the **renormalisation** of the following process:





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Field Theory Renormalisation: What are the loops

What physical process do the loops



correspond to? Trajectory intersecting itself (contract along wriggly line):





Renormalisation: What are the loops

What physical process do the loops



correspond to? Trajectory intersecting itself twice (contract along wriggly line):



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Results

Focus on first moment of sausage volume as a function of time.

- In one dimensions: Length covered proportional to square root of time, $\langle \alpha \rangle = \frac{\tau}{\kappa} 4 \sqrt{\frac{tD}{\pi}}$. Exact amplitude!
- In two dimensions: Area covered linear in time, t (modulo logarithmic corrections, t/ln(t)).
- In general: $\langle a^m \rangle \propto t^{md/2}$.
- Finite size scaling can be done explicitly.
- In three dimensions and higher: Volume linear in time, t.
- ... random walker may never return.
- Well known results (Leontovich and Kolmogorov, Berezhkovskii, Makhnovskii and Suris)...
- ... but, hey, what a nice playground for field theory (fermionicity, renormalisation, calculating moments easily ... [sort of]).

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Thank you!

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