Studies of ERM Models with Correlated Disorder

by Tom Folgmann

Bachelor Thesis Presentation, 2024

What is ERM?

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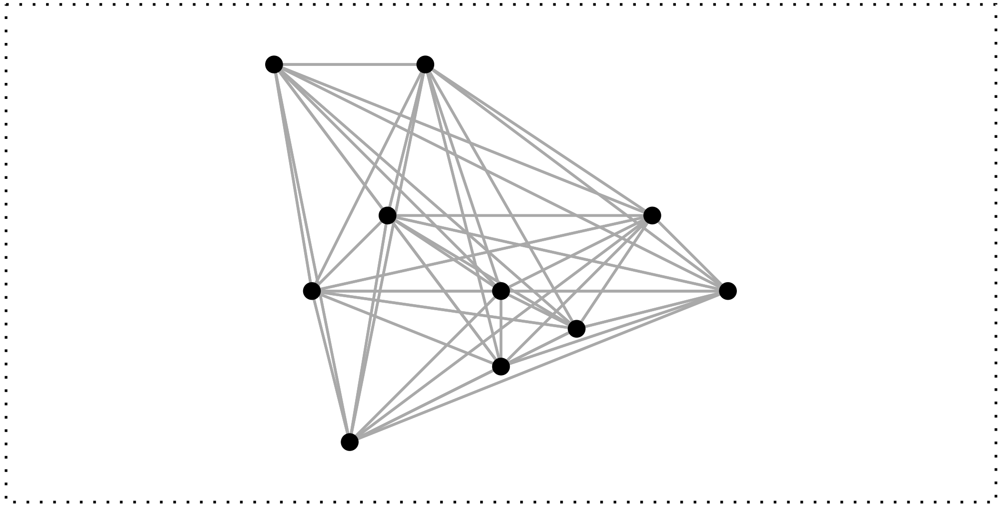

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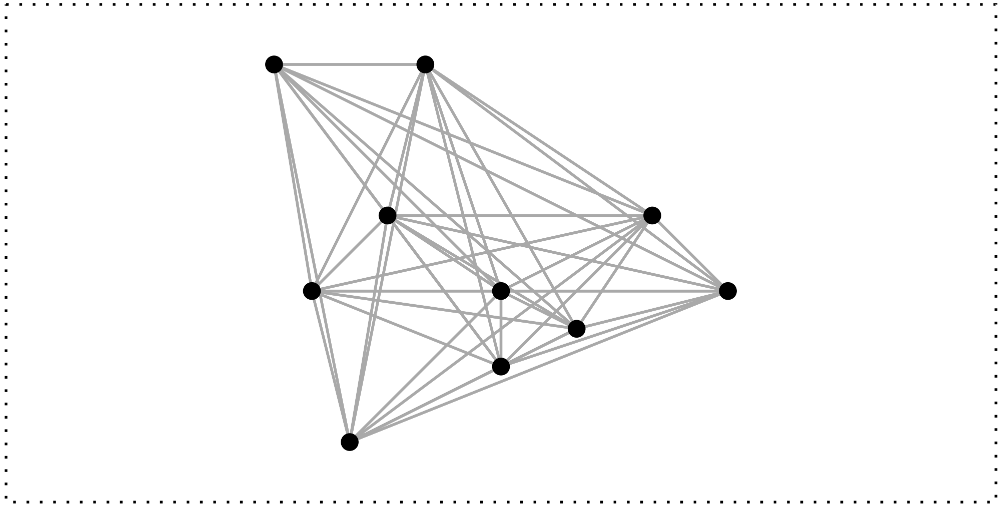

A system with $N \in \mathbb{N}$ (related) particles can be described by a mathematical *Graph*.

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.. special case is the *Adjacency Matrix* A, where $w_{i,j} \in \{0, -1, 1\}$.

Definition of the ERM Laplacian Matrix

In the ERM model the Laplacian matrix is defined as

$$\tilde{U}(f,r) := \begin{pmatrix} \Sigma(f,1) & -f_{12} & \dots & -f_{1N} \\ -f_{21} & \Sigma(f,2) & \dots & -f_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ -f_{N1} & -f_{N2} & \dots & \Sigma(f,N) \end{pmatrix},$$

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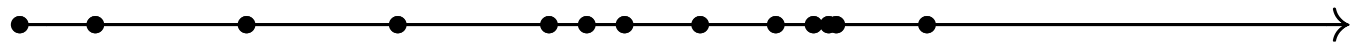

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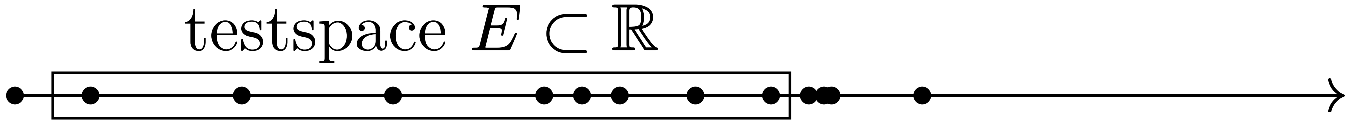

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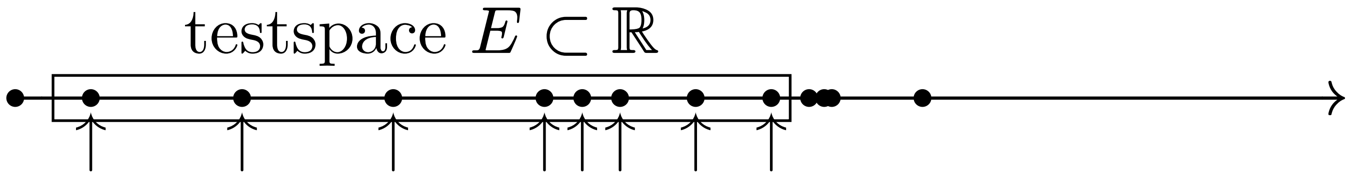

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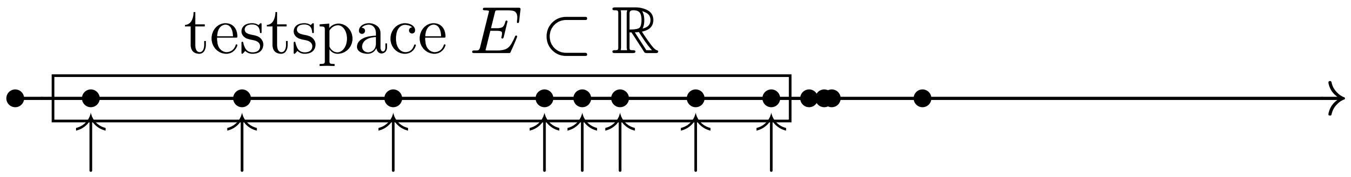

... results in an (unnormalized) density function

$$E \mapsto \sum_{i \in [p]} \delta_{\Lambda_i}(E) \qquad \in \{0, p\}$$

The Resolvent Eigenvalue Approximation

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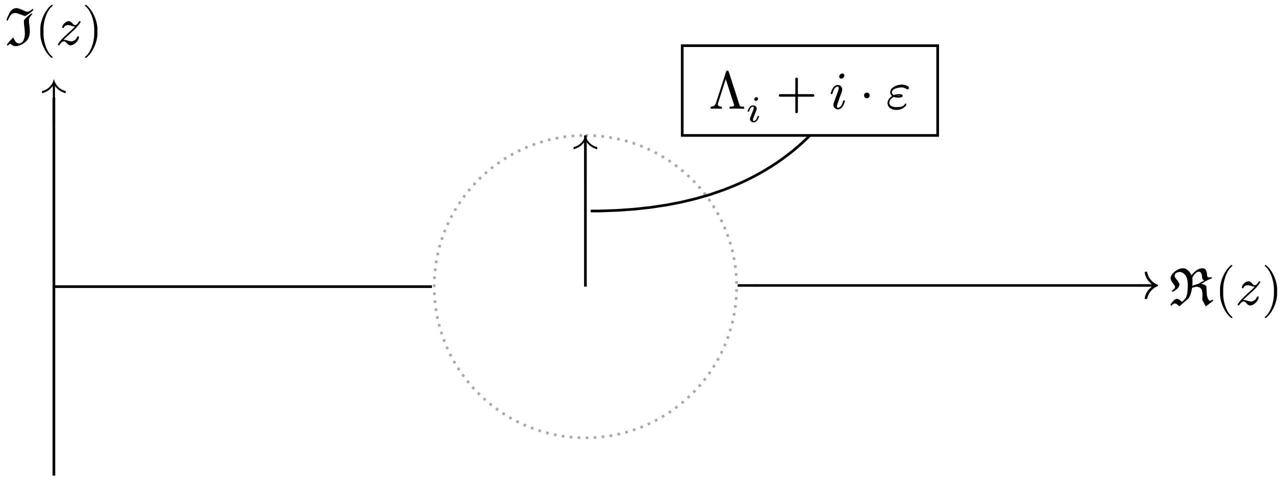

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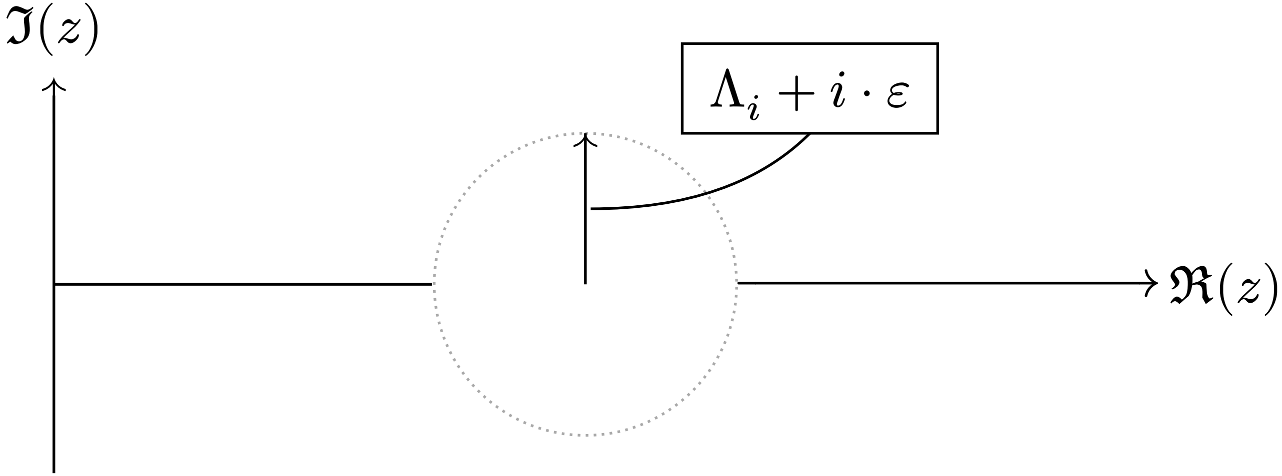

$\hookrightarrow$ Usecase is the resolvent with a singularity at Λ_i.

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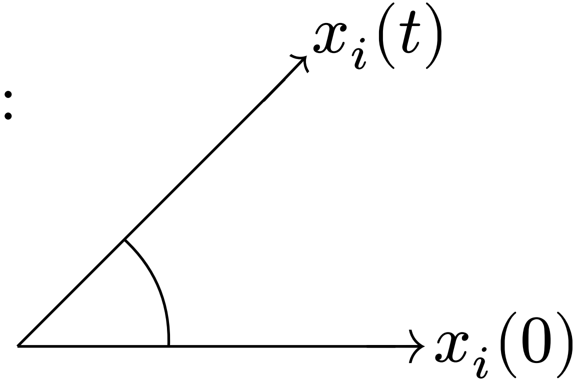
.. looking at the behaviour with regard to the initial conditions:

$$\left(\frac{d}{dt}\right)^2 \langle x_i(t), x_i(0)\rangle = -\tilde{U}(f, i \mapsto x_i(t))_{i,j} \cdot \langle x_j(t), x_i(0)\rangle.$$

In a visual approach $\langle x_i(t), x_i(0)\rangle$ represents:



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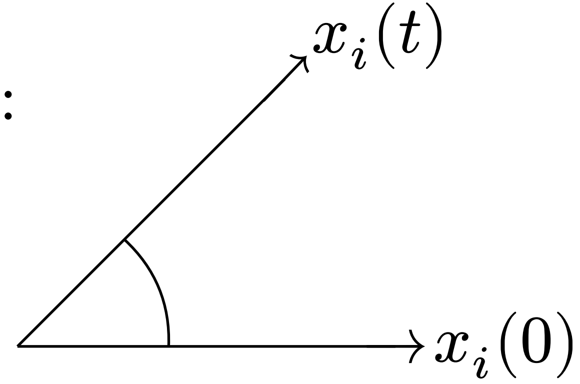

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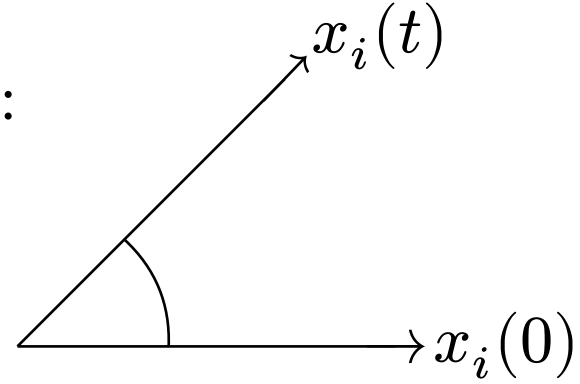

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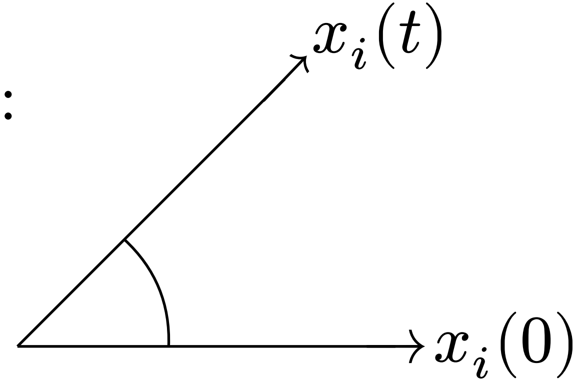

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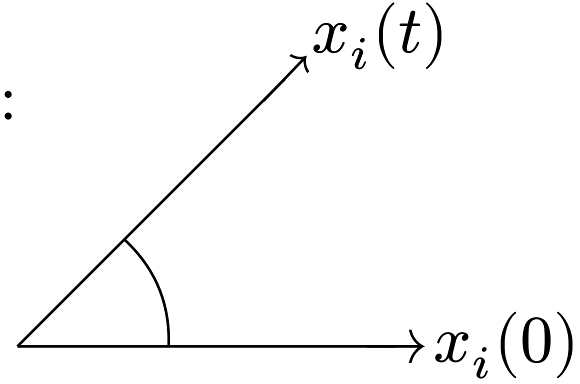

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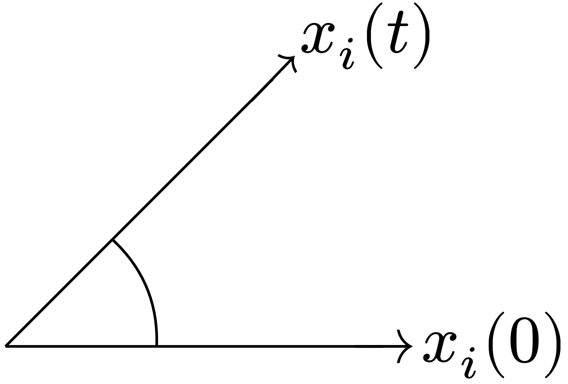

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$$\left(\mathcal{L}F_{j,i}\right)(s) = \pm \frac{1}{\tilde{U}(f, x^*(t))_{i,j} - \delta_{ij} \cdot \lambda_i^2}.$$

[6] With $x^*(t) = \left(i \mapsto x_{i(t)}\right)$ and $F_{j,i}(t) := \langle x_j(t), x_i(0)\rangle$.

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Ev. step	**Meaning**
R	Random variable, abstract
$R(\omega)$	Vector of time dep. pos.
$R(\omega)_i$	i-th particle position, time dep. path
$R(\omega)_i(t)$	Position of i-th particle at time t

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This is already a good starting point to understand our *Correlated Disorder* modification!

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[7] Expansion to a functional can be argued, see thesis p. 19.

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- The *moment generating function* $Z_{z,R_\omega}[J]$. It requires the *force field* J.

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Definition 2.22. External Field Shift.

For $R : \Omega \to V_{d,N}$ and $\Phi \in \mathbb{F}_{d,N}$ we define

$$J \mapsto -\frac{1}{2} \cdot S^{(0)}_{z,R_\omega}(\Phi) + \int_{\mathbb{R}^d} J(x) \cdot \Phi(-x) + J(-x) \cdot \Phi(x)\, \lambda(dx)$$

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$$\hookrightarrow \quad \frac{\delta}{\delta J(x)} S^{(0)}_{z,R_\omega}[\Phi] = \mathring{i} \cdot \Phi(-x).$$

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→ Looking at different Taylor expansion terms yields different integrals.

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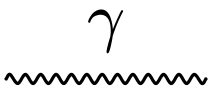

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.. possible connections of these edges are given by *vertices*:

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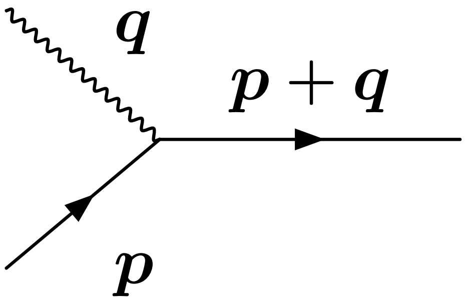

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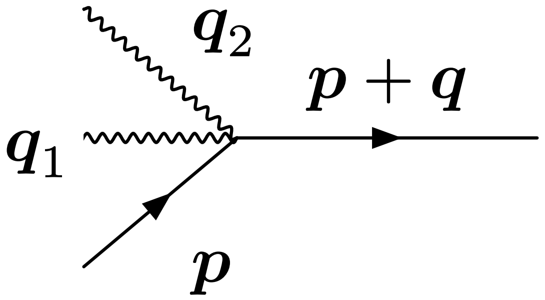

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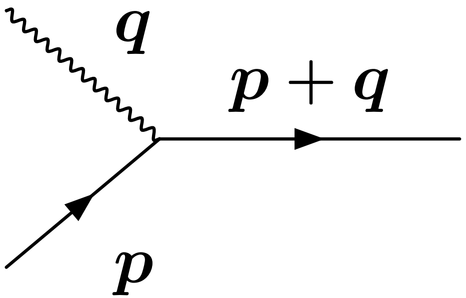
Feynman Diagrammatics - Vertices



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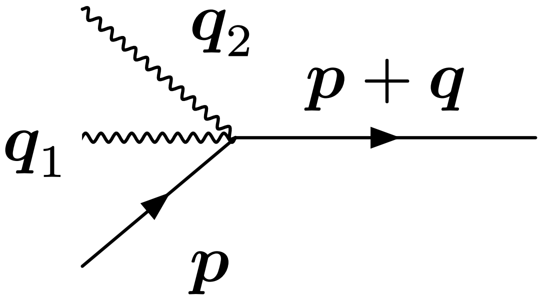

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.. which completes the set of Feynman rules.

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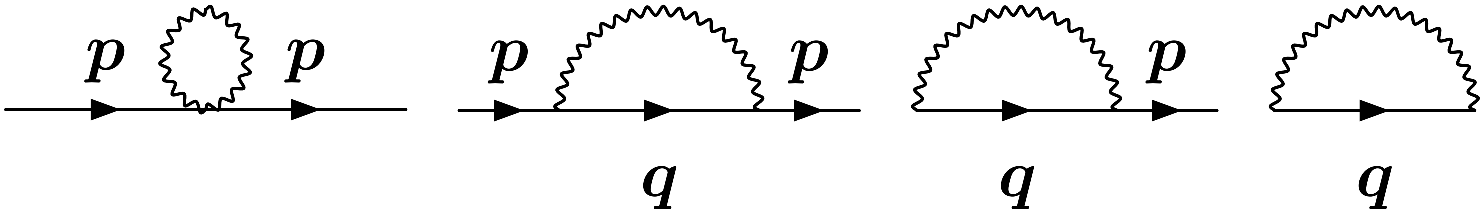

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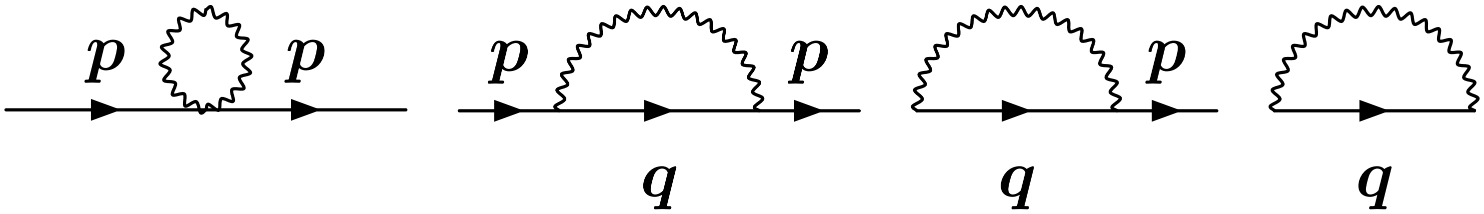
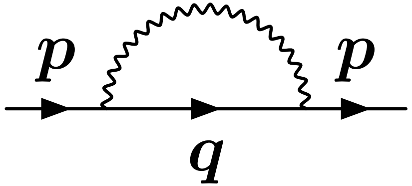


.. represented diagrams are *irreducible*: $Z_{z,R_\omega}[J] = \exp\Big(\sum_{C\in\mathcal{C}} C\Big)$.

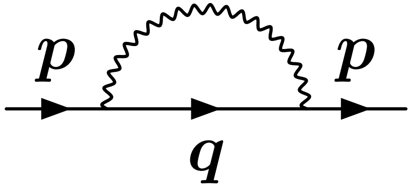
Integral representations[12]

[12] Attention! The terms have been simplified. For more details see Thesis sec. 2.4.2.

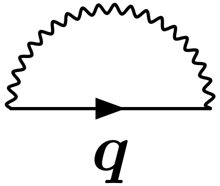
Integral representations[13]



$$= \frac{G_0(\boldsymbol{p}, z)^2}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(\boldsymbol{q} - \boldsymbol{p}, z) \cdot \mu_z(\boldsymbol{p}, -\boldsymbol{q})^2 \, d\boldsymbol{q},$$



$$= -\frac{2 \cdot G_0(\boldsymbol{p}, z)}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(\boldsymbol{p} - \boldsymbol{q}, z) \cdot \mu_{z(\boldsymbol{p}, -\boldsymbol{q})} \, d\boldsymbol{q},$$



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Main question to solve:

How can we include *structure* in our probability density?

The (radial) Particle Distribution Density

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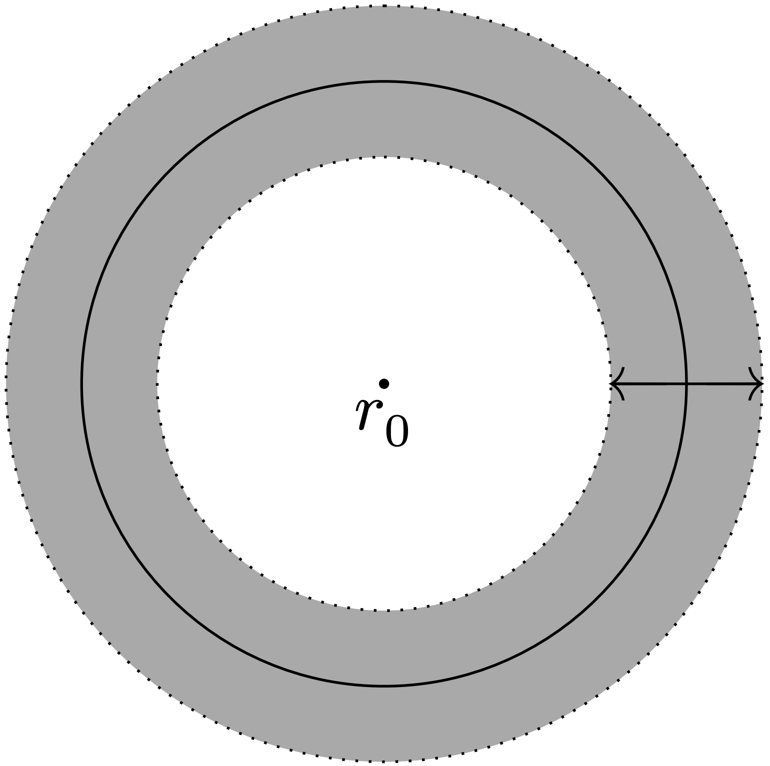
To calculate possibility of finding particles near a given reference r_0 we used the *radial distribution function*

$$g_{r_0}(r) = \int_{\mathbb{R}^d} \rho_N^{(2)}(r_0 + r, r)\, dr,$$

while $\rho_N^{(2)}$ reflects integration of $\exp(-\beta \cdot H(r, \cdot))$ for remaining particles.



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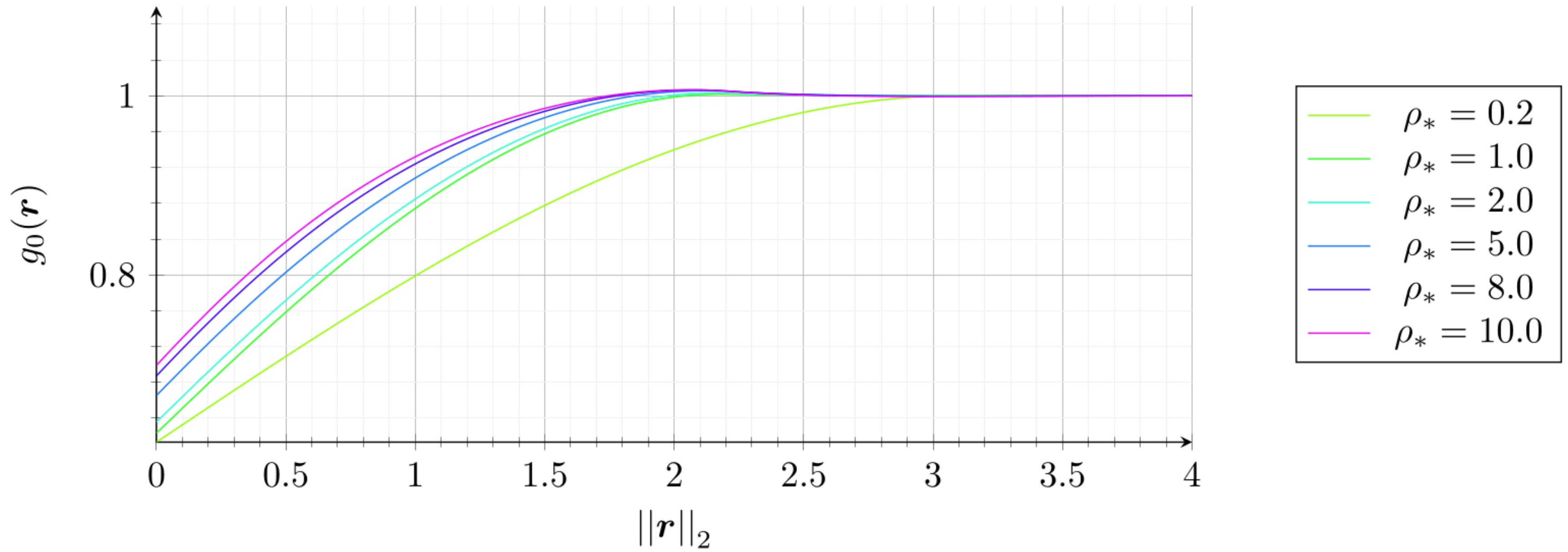
.. namely given by

$$S_*(\boldsymbol{q}) = 1 + \int_{\mathbb{R}^d} (g_0(\boldsymbol{r}) - 1) \cdot e^{\mathring{\imath} \cdot \boldsymbol{q} \cdot \boldsymbol{r}} \, d\boldsymbol{r}.$$

What does g_0 look like?[14]

[14]Looking at a soft sphere model, see later.

What does g_0 look like?[15]



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Resulting in the Static Structure Factor

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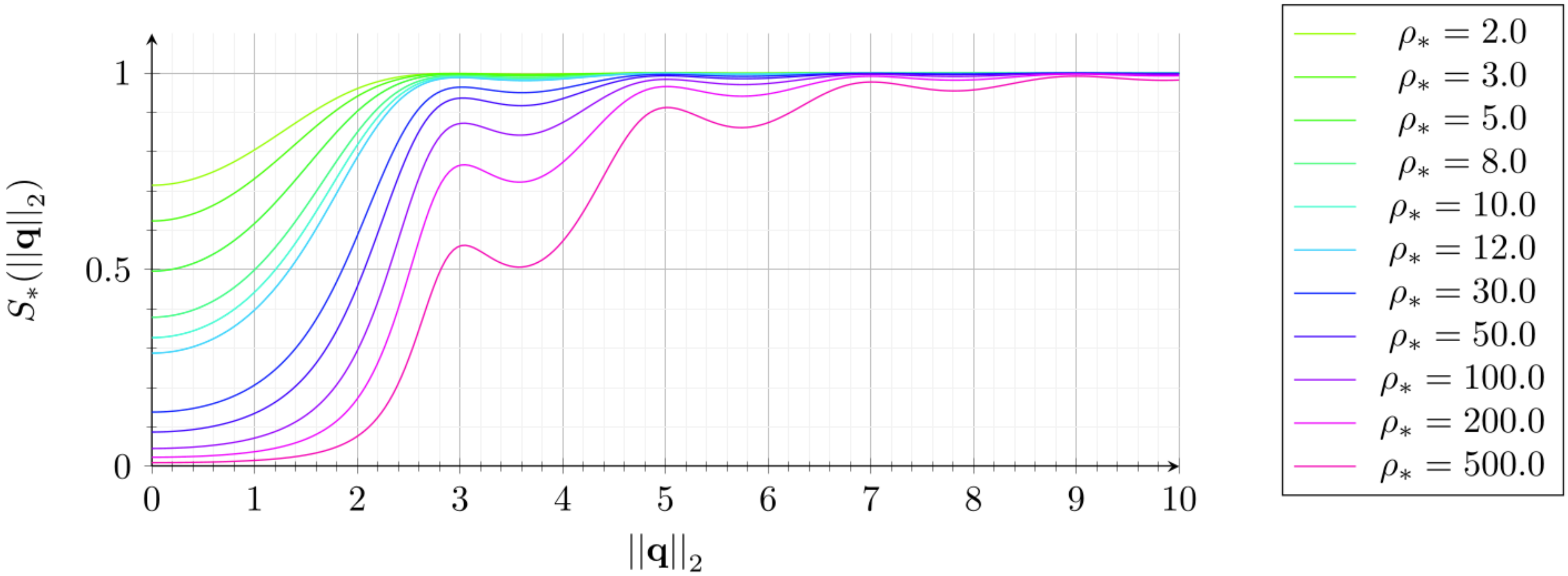

Where did we implement this, what did it change?

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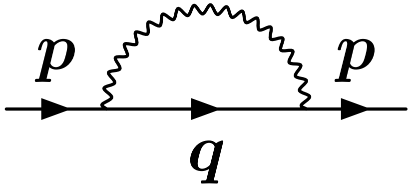

$$= \frac{G_0(\boldsymbol{p}, z)^2}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(\boldsymbol{q} - \boldsymbol{p}, z) \cdot \mu_z(\boldsymbol{p}, -\boldsymbol{q})^2 \cdot S_*(\boldsymbol{q})\, d\boldsymbol{q},$$

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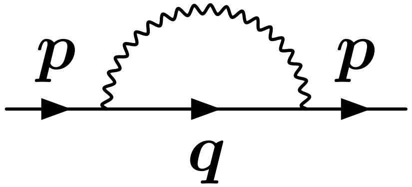

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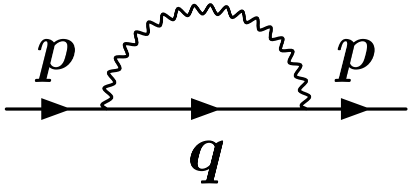

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This also affects the Self-Energy:

$$\Sigma^{(1)}_{S_*}(\boldsymbol{p}, z) = \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(\boldsymbol{q}) \cdot G_0(\boldsymbol{p} - \boldsymbol{q}, z) \cdot S_*(\boldsymbol{q})\, d\boldsymbol{q}.$$

Can we in any way compare our results?

The Approach of Martin-Mayor

The Approach of Martin-Mayor

Here, a *superposition approximation* was used:

$$\frac{1}{\left|V_{d,N}\right|} \cdot \exp(-\beta \cdot U(r)) \approx \frac{1}{\left|V_{d,N}\right|} \cdot \exp\left(-\beta \cdot \sum_{i \in [N-1]} u(r_i - r_{i+1})\right)$$

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$$\exp(-\beta \cdot U(r)) = \exp\left(-\beta \cdot \sum_{(i,j) \in [N]^2} u(r_i - r_j)\right).$$

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An implementation of $r \mapsto \frac{\exp(-\beta \cdot \sum ..)}{|V_{d,N}|}$ is done:

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This has an explicit approximation built into the spring function!

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- We explicitly did not approximate the spring function.
- We did not change the zeroth order term in the propagator.

What did a numerical model show?

Analytical Foundation

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We chose a *step function* for the spring mapping:

$$\mathbb{R} \ni r \mapsto f_a^{(num)}(r) = \begin{cases} 1 \text{ if } r < a, \\ 0 \text{ else.} \end{cases}$$

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$$V_{d,N} \ni R \mapsto U_a^{(num)}(R) = \sum_{(i,j)\in[N]^2} \begin{cases} \frac{1}{2} \cdot \left(\|R_i - R_j\| - a\right)^2 \text{ if } \|R_i - R_j\| < a, \\ 0 \text{ else.} \end{cases}$$

Results using the Hypernetted Chain

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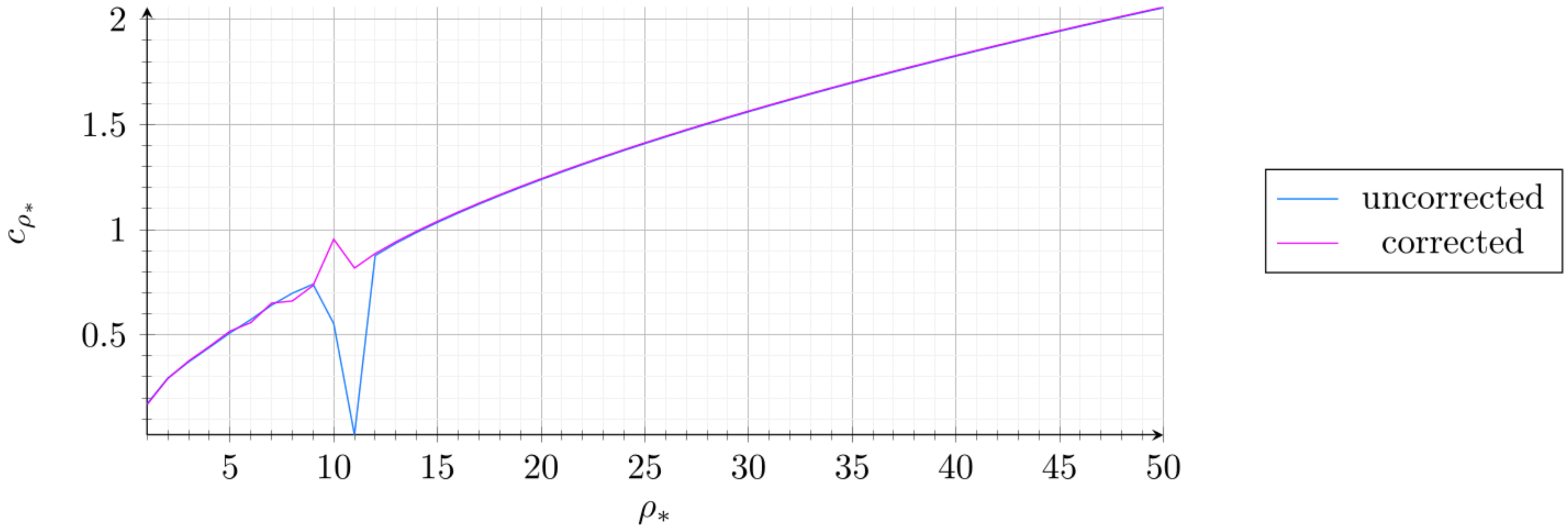

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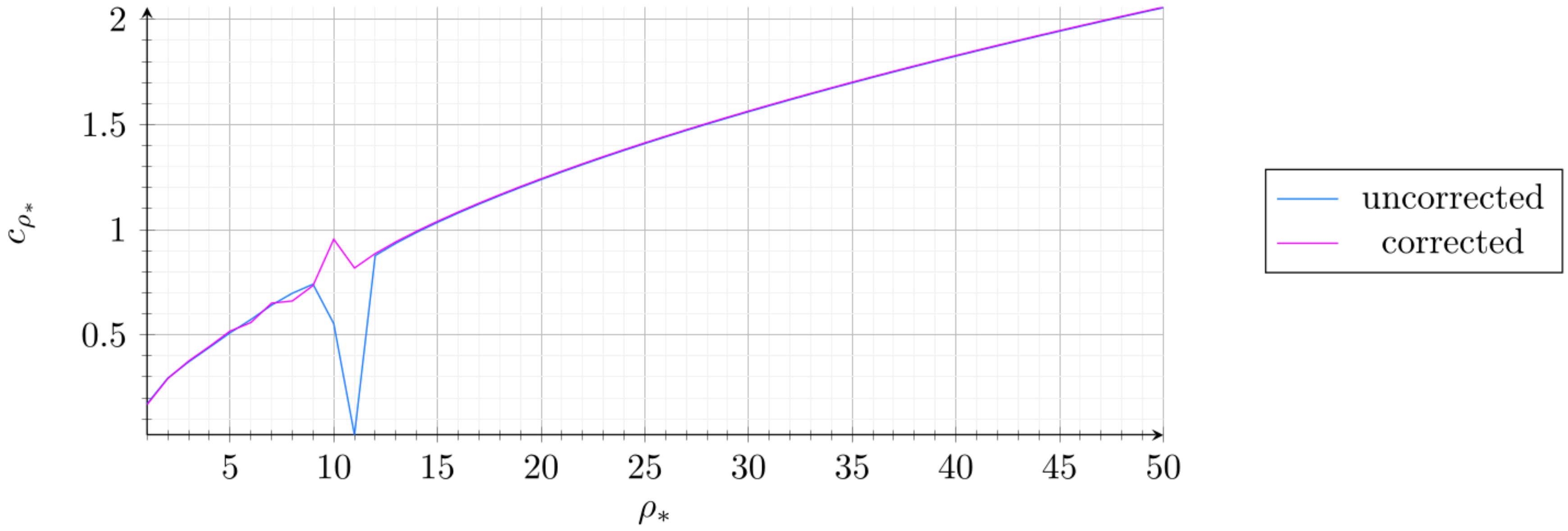

→ Sadly no major differences in the velocity of sound noticeable.