

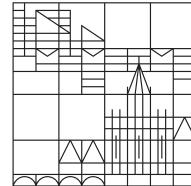
Studies of ERM Models with Correlated Disorder

Bachelor Thesis

submitted by
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at

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Zwischen zwei Welten

Gedämpft nehme ich die Geräusche wahr, die um mich herumschwirren im verschwommenen Farbenmeer. Alles scheint dumpf, fast pausiert zu sein- die Bewegungen der Blase, die mich umgibt, sind langsam und bedacht, doch unaufhaltsam und bestrebt. Ich strecke den Finger aus um nach ihr zu fühlen, sie zu ertasten, die Wand, die mich umschließt, doch mein Arm scheint lang genug nicht zu sein, kläglich fällt des Fingers Spitze zurück zu mir selbst. Unverändert, mein Tun nicht zur Kenntnis nehmend, bewegt sich der Schleim um mich herum fort und erleuchtet in manchen Sekunden die Augen blendend hell meinen Blick. Vor mir liegt eine Welt, die mir noch fremd erscheint, während sich hinter mir alles aufhält, das ich einst mein Leben nennen konnte. Wie ich den KKkkkKkkKKKK

TRY ERROR CORRECTION DECRYPTING KKKkopf zu dieser Welt hindrehe, fängt in selber Dynamik die Umgebung an sich zu bewegen, als würde ich Kontrolle übernehmen über den Schleim, der eben noch unbeteiligt sich frei bewegte: Ich sehe mich wieder im Spiegel der Vergangenheit, klar und doch weit entfernt. Erinnerungen weckt das Getose jenseits der Scheibe, dass mir die Worte fehlen.

Ich drehe mich erneut und blicke voraus, hinein in die Welt, die sich vor mir ausbreitet und meine Augen erleuchtet- Wärme verspürt meine Haut, als würde sie von ihr emittiert werden, doch bleibt mein Körper in fortwährender Unbeweglichkeit. Ich erkenne mich wieder, schwebend, schauend, horchend, fühlend.

Zwischen zwei WeLten.

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... static sound beholds your ear, flickering lights alarm your eyes, soft warmth tickels your skin, a bitter taste lies upon your tongue. You know it is time ...

goodbye.

↪ DANKSAGUNG ↵

This thesis is dedicated to my time in Konstanz and all the experiences I have been able to gather during that period of my life.

Some sections of this thesis may appear lengthy and have a sticky feel to them. This is due to the amount of work I put into disassembling what was already constructed by experts in this field who are highly skilled physicists and mathematicians. It became a huge challenge for me at some points and I cannot wait to be as fluent as many authors of the papers and books I have read appear to be. But for now I have to try to do a detailed analysis of every component to thoroughly convince myself of physical understanding and to feel the fresh breeze of founded research.

Without the technology I am able to savour, the time of writing would have been much more of a struggle. Open sourced tools like vim and L^AT_EX Julia and Zathura made my days a breeze and joy. And this is what I adore about the world, the human being and spirit; Its ability to create greatness and share it with everyone.

This also is what each and every professor and teacher did for me, beginning in the first semester with lectures such as *Analysis 1* with professor Junk and *Lineare Algebra 1* with professor Schweighofer, whose value only later on became clear to me. There were so many other valuable lectures and courses I have been able to attend, I especially think of the *mathematische Grundlagen der Quantenmechanik* by professor Denk, or follow along, I think of the *Theorie und Numerik partieller Differentialgleichungen* by professor Junk and Gmeineder. As a student of physics I naturally also attended great and demanding classes in IK, where I learned from professor Fuchs whose team build the foundation of this thesis, mainly taught to me by their member Florian Vogel. Despite the challenges those classes have brought to me, I am grateful that I had the opportunity to attend and learn from them. They greatly shaped my way of thinking and understanding of everything surrounding me.

But now I wish to make place for some of the most thoughtful, inspiring and loving people I have met during my studies.

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To Arto, who brought new warmth into my life, who challenged and changed the way I think and act. Who taught and brought me culture of france, art and joy, espaecially in times of the *Franzosen-Action*. And you wondered beneath the stars, what value our friendship would have..

you are the most valuable friend I have. This chapter really is .. *powered by bro.*

And to you Άρτεμις. I was not prepared to meet you, and yet the subway of HD took off. I still see you standing beneath the public library with a giant hat, a big smile and glowing eyes. During our time you truly made me grow and supported me with all your heart. Without you, life would have been so much of a different story. *Σάγαπώ αγάπη μου.*

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As I am sitting here by myself, writing the last paragraphs, a truly, truly dense tear runs down my cheek. Without the miracle of you all I would have never loved and enjoyed life as much as I did.

“Don’t hide away - come out and play.”

Tom Folgmann

Konstanz, 26.02.2024 and July 2024

↪ ABSTRACT ↵

In this thesis the impact of correlated disorder in particle positions is discussed in the context of the euclidean random matrix model. It consists of an isotropic system of N particles in a d -dimensional space where the dynamics are given by a pair interaction spring function f . It is furthermore frozen in time and in an athermal state with a reference system. Hereby results a random matrix $\tilde{U}(f, R)$ whose spectral properties are discussed using a field theoretical approach. After introducing the Dyson formalism and deriving the feynman rules, the static structure factor S_* is introduced, based on the Fourier transform of the radial particle distribution function $g_0 - 1$. Using a self consistent Born approximation, the one loop self energy $\Sigma^{(1)}$ is corrected to $\Sigma_{S_*}^{(1)}$ and the corresponding Dyson equation is derived.

By its numerical solution to an example of a three dimensional space using a Heaviside step function as the spring function, the impact of the static structure factor on the speed of sound is discussed. It is shown that the structure factor is stable for all tested densities but has no significant impact on the speed of sound. The dispersion relation is shown to be nearly unchanged for all densities. It is also discussed when the model reaches physical applicability by a fully positive dispersion relation. Lastly the results are compared to and verified by a gaussian radial distribution.

→ ZUSAMMENFASSUNG ←

In dieser Arbeit wird der Einfluss korrelierter Unordnung in Partikelpositionen im Kontext des euklidischen Zufallsmatrixmodells diskutiert. Dabei handelt es sich um ein isotropisches System von N Teilchen in einem d -dimensionalen Raum, dessen Dynamik durch eine Federfunktion der Paarwechselwirkung gegeben und zeitlich athermisch eingeforen ist. Daraus resultiert eine Zufallsmatrix, deren spektrale Eigenschaften unter Verwendung eines feldtheoretischen Ansatzes diskutiert werden. Nach Einführung des Dyson-Formalismus und Herleitung der Feynman-Regeln wird der statische Strukturfaktor S_* eingeführt, welcher auf der Fouriertransformation der radialsymmetrischen Verteilungsdichte der Teilchenpositionen $g_0 - 1$ beruht. Unter Verwendung der selbstkonsistenten Born Näherung wird die Selbstenergie im Einklang dessen korrigiert und die entsprechende Dyson-Gleichung hergeleitet. Die Feynman-Regeln werden ebenfalls korrigiert.

Durch die numerische Lösung der Dyson Gleichung im Beispiel eines dreidimensionalen Raums und einer Stufenfunktion als Federfunktion wird der Einfluss des statischen Strukturfaktors auf die Schallgeschwindigkeit diskutiert. Dabei wird gezeigt, daß zwar der Strukturfaktor für alle getesteten Dichten stabil im positiven Bereich liegt, jedoch keinen signifikanten Einfluss auf die Schallgeschwindigkeit ausübt. Die Dispersionsrelation wird für alle Dichten als nahezu unverändert gezeigt. Ebenfalls wird die physikalische Anwendbarkeit im Hinblick auf die Positivität der Dispersionsrelation diskutiert. Abschließend wird das Modell mit einer gaußschen Radialverteilung verglichen und das Ergebnis verifiziert.

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↪ INTRODUCTION ↵

Chapter 1

Generally speaking we describe a classical system of $N \in \mathbb{N}$ particles using the *phase space* $\Gamma_1 \times \Gamma_2 \subset (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ of *positions* and *moments*, and a hamiltonian function $\mathcal{H} : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow \mathbb{R}$. Its properties determine if the system describes a liquid, solid or gas. If the function can be independently split into a kinetic and potential part, i.e. $\mathcal{H}(p, r) = T(p) + U(r)$, integral factorization can already be done via

$$\int_{\Gamma_1 \times \Gamma_2} \exp(-\beta \cdot \mathcal{H}(p, r)) \lambda(d(p, r)) = \int_{\Gamma_1} \exp(-\beta \cdot T(p)) \lambda(dp) \cdot \int_{\Gamma_2} \exp(-\beta \cdot U(r)) \lambda(dr).$$

The factor $\beta := (k_B \cdot T)^{-1}$ can be interpreted as an inverse temperature of the system, with k_B being the Boltzmann constant. This already means that the Boltzmann density $(p, r) \mapsto \exp(-\beta \cdot \mathcal{H}(p, r))$ is divided into a product of two densities P and Q on Γ_1 and Γ_2 respectively. Application of $\int_{\Gamma_1} 1 P = 1$

$$\int_{\Gamma_1 \times \Gamma_2} \exp(-\beta \cdot \mathcal{H}(p, r)) \lambda(d(p, r)) = 1 \cdot \int_{\Gamma_2} \exp(-\beta \cdot U(r)) \lambda(dr)$$

In this state an expansion on the position arguments can be done, such that by the potential U defined rigid equilibrium positions $r_0 \in \text{critP}(U)$ are assumed, from which small deviations ϕ lead to yet another expansion of the potential energy [1]. This approach is also used in the Euclidean Random Matrix (ERM) model.

The ERM model was introduced in 1999 by Mézard, Parisi and Zee [2] and has since then been studied by Grigera [3] and others. It introduces an interaction matrix $\tilde{U}(f, R)$ which is given by

$$\tilde{U}(f, R) = \delta_{ij} \cdot \sum_{(i,j) \in [N]^2} f(R_i - R_j) - f(R_i - R_j).$$

This Laplacian form is motivated due to requirement of a conservation law $\sum_{j \in [N]} \tilde{U}(f, R)_{i,j} = 0$, otherwise simply the pairs $f(R_i - R_j)$ would populate the matrix' entries [3]. Its appearance can be motivated by graph theory, which we will discuss in the next sections. The application of the model can be seen in vibrational analysis of glasses or vibrations in DNA [3].

The pair interaction function f is set with regard to the potential U , which in our model is a summation of pair potentials u following $U(R) = 1/2 \cdot \sum_{i,j} U(R_i - R_j)$. Hereby only rotational invariance (and therefore a scalar character in f) and Fourier transformability are required, otherwise the potential u and respective f can be chosen freely [3]. Its application can be seen

in the Taylor series of the positional component to the hamiltonian function \mathcal{H} :

$$\begin{aligned} \int_{\Gamma_2} \exp(-\beta \cdot U(r)) \lambda(dr) &\stackrel{r \mapsto r_0 + \phi}{\approx} \int_{\Gamma_2} \int_{\Gamma_2} \exp(-\beta \cdot U(r_0 + \phi)) \lambda(d\phi) \lambda(dr_0) \\ &\approx \int_{\Gamma_2} \int_{\Gamma_2} \exp\left(-\beta \cdot \underbrace{\left(U(r_0) + dU(r_0)(\phi)\right)}_{\text{negl.}} + \underbrace{\frac{1}{2} \langle HU(r_0) \cdot \phi, \phi \rangle}_{=0 \rightarrow \text{ERM}}\right) \lambda(d\phi) \lambda(dr_0). \end{aligned}$$

Hereby the ERM model is introduced by the second order term in the Taylor series of U and the Hessian matrix HU of U at r_0 . Its critical idea is the expansion of the positions to equilibrium states and small variations around them. This can be done in amorphous solids [1].

The key observation is that up until now the model was discussed in the context of *uniformly* distributed particle positions $r \mapsto 1/|\Gamma_2|$, i.e. matrix elements [3, 4]. Although some considerations have been done by Martin-Mayor in [5], we provide an enhanced view on particle correlations in ERM by introducing the static structure factor into the Feynman rules. This firstly introduces structural aspects into the mathematical formalism of ERM.

It is then particularly interesting to see how the corrected model compares to the current state. We will do this by looking at a specific example of a N particle system in a soft sphere potential.

↪ THE SYSTEM ←

Chapter 2

Interacting particles in a physical system can be neatly described by diagrams and graphs, in which nodes represent particles and edges the interactions between them. This can be visualized on the two dimensional plane, which incidentally offers a very familiar and intuitive playground, often resulting in stunning images:

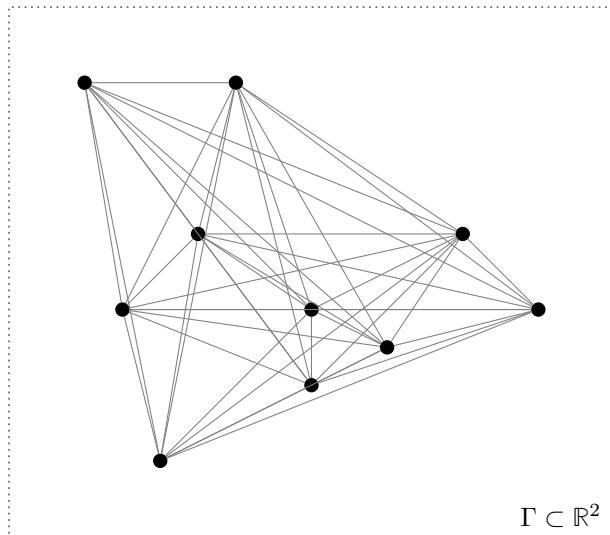


Figure 1: Graph representation of a physical system with $N = 10$ particles in \mathbb{R}^2 .

To be able to describe this almost always abstract world, we need to introduce a few mathematical utilities and principles.

2.1 Mathematical Principles

To start off, a mathematical description of the particle system above is given by a mathematical object called a *graph*.

Definition 2.1. Graph.

A graph G is a pair $G = (V, E)$, where V is a set of elements called *vertices* and $E \subseteq V^2$ is a set of edges, each of which is a pair of vertices. We call G *undirected* if $(v_1, v_2) \in E \implies (v_2, v_1) \in E$. We say v *initiates* (and is adjacent to) w if $(v, w) \in E$ and v *terminates* w if $(w, v) \in E$, in short $v \sim w$ and $w \sim v$ respectively.

Its properties can be analysed and characterized. For example, if we know the amount of particles in a box, we could ask how many other particles are influenced by the existence of our reference particle. In the language of mathematics this is called the *degree* of a node.

Definition 2.2. Degree and Degree Matrix.

Let $G = (V, E)$ be a graph. The *degree* of a node $v \in V$ is the number of edges incident to v , namely the cardinality of the set $\{u \in V : (u, v) \in E \vee (v, u) \in E\}$. The *degree matrix* $D(G)$ of G is then $D(G) = \text{diag}(d_1, \dots, d_n)$ with d_i being the degree of the i -th node.

Since our particle interaction will be undirected, we do not have to distinguish between the initiation and termination of a particle. Later on this will be given by a symmetry $f(x) = f(-x)$ in the pair interaction function [3, 4]. The value of f , namely the strength of interaction, can be mathematically encoded in the *weight matrix* of a graph.

Definition 2.3. Weight Matrix.

We call $G = (V, W)$ a *weighted graph* if $|V| < \infty$ and $W : V \times V \rightarrow \mathbb{R}$ is a function. If W is symmetric and $W(v, v) = 0$ for all $v \in V$, then we call G an *undirected weighted graph*. The *underlying graph* of G is then given by its set of edges $E = \{(u, v) \in V \times V : W(u, v) \neq 0\}$. If $\forall v, w \in V : W(v, w) = 1$, W becomes the adjacency matrix A .

From these definitions we can already construct a matrix that will be very prominent in our model, the *laplacian matrix*.

Definition 2.4. Laplacian Matrix.

Let $G = (V, E)$ be a graph. The (unnormalized) *Laplacian matrix* $L(G)$ of G is then given by $L(G) = D(G) - A(G)$. If $G_* = (V_*, E_*, W)$ is a weighted graph, then $L(G_*) = D(G_*) - W(G_*)$.

The laplacian matrix in its entries will encode the interactions between particles i and j . It is also related to differential geometry and the discretized Laplace operator, but we will not go into detail here. For directed graphs it is also interesting to characterize *if* and *how* particles are connected. This can be done by the *incidence matrix*.

Definition 2.5. Incidence Matrix.

Let $G = (V, E)$ be a graph. The *incidence matrix* $B(G) \in (|V| \times |E| \rightarrow \{0, \pm 1\})$ for $v \in (|V| \rightarrow V)$ and $e \in (|E| \rightarrow E)$ is defined as

$$B(G)_{i,j} = \begin{cases} 1 & \text{if } v_i \text{ is the initial node of } e_j, \\ -1 & \text{if } v_i \text{ is the terminal node of } e_j, \\ 0 & \text{otherwise.} \end{cases}$$

If G a weighted graph, then instead of ± 1 we have $\pm \sqrt{W(v_i, v_j)}$.

Practically for our model every particle is connected with each other in a symmetric way. This means that $w_{ij} = w_{ji}$ for a weight function $w : |V|^2 \rightarrow \mathbb{R}$. In an example with $V = \{a, b, c\}$ and $E = \{(a, b), (b, a), (a, c), (c, a), (b, c), (c, b)\}$ the incidence matrix would therefore look like

$$G \cong \begin{array}{ccc} & \bullet & \\ & / \quad \backslash & \\ w_{ca} & & w_{bc} \\ \backslash \quad / & & \\ \bullet & & \bullet \\ & w_{ab} & \end{array} \implies B_G = \begin{pmatrix} \sqrt{w_{ab}} & -\sqrt{w_{ab}} & -\sqrt{w_{ac}} & \sqrt{w_{ac}} & 0 & 0 \\ -\sqrt{w_{ab}} & \sqrt{w_{ab}} & 0 & 0 & \sqrt{w_{bc}} & -\sqrt{w_{bc}} \\ 0 & 0 & -\sqrt{w_{ac}} & \sqrt{w_{ac}} & -\sqrt{w_{bc}} & \sqrt{w_{bc}} \end{pmatrix}.$$

It can be shown that $L = B \cdot B^\top$ and $L = D - W$ are equivalent [6].

Moving on, the modelling of glasses is founded on randomly positioned particles which are proportionally to their displacement from their equilibrium state impacted by a harmonic restoring force. Evaluating their mean with respect to equilibrium positions and displacements yields a theoretical prediction that can be compared to experimental data or other established theories, for example with respect to vibrations in glasses [3]. To mathematically describe the randomness of particle positions within those graphs, we introduce the concept of *probability spaces*.

Definition 2.6. Random Variables on Propability Spaces.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a measure space and (S, \mathcal{S}) a measurable space. We call \mathbb{P} a *probability measure* on \mathcal{A} if $\mathbb{P}(\Omega) = 1$. A *S-valued random variable* then is a \mathcal{S} -measurable function $X : \Omega \rightarrow S$, i.e. for all $A \in \mathcal{S}$ we have $X^{-1}(A) \in \mathcal{A}$.

This concept seems fairly abstract, but it is a very powerful tool used throughout this thesis. It becomes more accessable when setting (S, \mathcal{S}) to $(\mathbb{R}^2, \mathcal{B}(\mathbb{R}^2))$ or even its trace on a box $\Gamma \subset \mathbb{R}^2$ with its Borel σ -algebra $\mathcal{B}(\Gamma)$. To more intuitively calculate expectancies throughout this paper we also introduce the *pushforward measure* given by a random variable X on \mathbb{P} .

Definition 2.7. Pushforward Measure of Random Matrices.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a measure space, (S, \mathcal{S}) a measurable space and $X : \Omega \rightarrow S$ a random variable. We define the *pushforward measure* \mathbb{P}_X on (S, \mathcal{S}) under X by $\mathbb{P}_X := \mathbb{P} \circ X^{-1}$.

Since we now start to talk about *integration*, one small note to notation should be made. Because within the thesis measures are of higher importance, we will explicitly denote which is currently used for notation. This will be done by writing μ at the end of the integral, i.e. $\int f \mu = \int f(x) \mu(dx)$. This expression now means integration with respect to the measure μ , from which the measure space is clear. The standard integral then is $\int f(x) dx = \int f(x) \lambda(dx)$, where λ is the Lebesgue measure.

The integral over $Y \subset \Omega$ regarding X can therefore be written as $\int_Y X \mathbb{P} = \int_{X(Y)} 1 \mathbb{P}_X$. If we consider particle position vectors, it is now far more intuitive talking about *where* the particles

randomly land (which is the $R(\omega) \in \Gamma$) than about the abstract process of random assignment $\omega \mapsto R(\omega)$.¹ Said integral becomes for $Y = \Omega$ the expectation value of X .

Definition 2.8. Expected Value and Variance.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space, (S, \mathcal{S}) a measurable space and $X : \Omega \rightarrow S$ a random variable. The expected value $\mathbb{E}(X)$ is then defined as

$$S \ni \mathbb{E}[X] := \int_{\Omega} X(\omega) \mathbb{P}(d\omega) = \int_S 1 \mathbb{P}_X.$$

The variance then is defined as the expected value of $\omega \mapsto (X(\omega) - \mathbb{E}(X))^2$.

Since we will talk a lot about the expectancy of products of random variables (which we will also refer to as *correlator*), this definition will become very prominent. If $[n] \rightarrow (\Omega \rightarrow S)$ is a collection of random variables, we will ask about how we can express the expectation value of their product in terms of simpler products, i.e. using the expectancy of *pairs* of random variables:

$$\mathbb{E}\left(\prod_{i=1}^n X_i\right) \stackrel{\text{What is the relation?}}{\longleftrightarrow} \sum_{p \in ?} \prod_{(i,j) \in p} \mathbb{E}[X_i \cdot X_j].$$

For a specific kind of probability measure this question can be explicitly answered: The normally pushforwarded measure of a random variable.

Definition 2.9. Normally Distributed Random Variable.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space and $(\mathbb{R}^d, \mathcal{B}(\mathbb{R}^d))$ a measurable space. A random variable $X : \Omega \rightarrow \mathbb{R}^d$ is called *normally distributed* if there exist $\mu \in \mathbb{R}^d$ and $\Sigma \in \mathbb{R}^{d \times d}$ positive definite and symmetric such that $\mathbb{P}_X = f_X \cdot \lambda$ with density $f_X(x)$ of the form

$$f_X(x) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \cdot \exp\left(-\frac{1}{2} \langle \Sigma^{-1} \cdot (x - \mu), x - \mu \rangle\right).$$

Within the theory of ERM we will find ourselves in the situation of having a normally distributed random variable, which will allow us to perturbatively produce Feynman graphs out of correlation functions. In physical terms this correlation function models the response of other particles positioning to one particle moving from its initial state. In the introduction we have already seen our idea of reparametrizing the phase space using two types of position arguments: the critical initial states r_0 and the shiftings ϕ . Both of them are measured by one probability measure \mathbb{P} , which can be split up into a product of two independent measures $\mathbb{P}_r \cdot \mathbb{P}_\phi$ thanks to the *stochastical independency* of the used random variable.

¹Funnily enough called the *law of the unconscious statistician*.

Definition 2.10. Stochastical Independency.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space and $X : I \mapsto (\Omega \rightarrow S_i)$ for a index set I and a family of measurable spaces (S_i, \mathcal{S}_i) . Then we call X a *stochastically independent* family of random variables if for any finite subset $I_0 \subset I$ the condition

$$\mathbb{P}\left(\bigcap_{j \in I_0} \{X_j \in B_j\}\right) = \prod_{j \in I_0} \mathbb{P}(X_j \in B_j).$$

for all $B_j \in \mathcal{S}_i$ holds. For $I = \{1, 2\}$ this simplifies to the condition

$$\mathbb{P}(\{X_1 \in B_1\} \cap \{X_2 \in B_2\}) = \mathbb{P}(\{X_1 \in B_1\}) \cdot \mathbb{P}(\{X_2 \in B_2\}).$$

Another assumption on our random variables is made, which assumes our physical system to be *frozen in time*. This means that we are only interested in one particular point in time and no statistical processes are happening. In physics, this setting also is referred to as *quenched disorder*.

Coming back to stochastical independency, having such simplifications at hand is of course not always the case, and sometimes there are no such formulars available or known. This will occur in our model when we introduce the corrected density function for the critical equilibrium positions of particles. In general one must find an alternative way of dealing and systemizing such products of random variables. In our case we will evade this problem by *gaussianizing* said density whilst knowingly making an error with this approximation, which will not be discussed.

For the seperation made in the introduction of $U(r_0 + \phi)$ we use the well known theorem of Taylor.

Theorem 2.1. Taylor's Theorem.

Let $f \in C^{p+1}(\mathbb{R})$ for $p \in \mathbb{N}_0$ and $x, h \in \text{Def}(f)$ such that^a $[x, x + h] \subset \text{Def}(f)$. Then there exists $\theta \in (0, 1)$ such that

$$f(x + h) = \sum_{k=0}^p \frac{1}{k} \cdot D_h^k f(x) + \frac{1}{(p+1)!} \cdot D_h^{p+1} f(x + \theta \cdot h).$$

The last summand will be namend $R_{p+1}(f, x, h)$ in this context.

^aWe denote an *interval* in \mathbb{R}^d as $[a, b] := \{a + t \cdot b : t \in [0, 1]\}$.

Its proof can be found in [7] or in any other analysis script and standard literature. Since we only use the first two derivatives of U in our model, by the theorem we introduce an error of $D_\phi^3 U(r_0 + \theta \cdot \phi)$ for some $\theta \in (0, 1)$. For our investigations we will not go into detail about its influence on our results.

Since we will thoroughly deal with Dirac functionals and measures when investigating the eigenvalues of the ERM matrix it is highly suggested to look into technical aspects, which are in short presented in the appendix.

What is of higher importance to introduce at this point is the *resolvent* of a matrix. It will be used to approximate the eigenvalues of the ERM matrix and states a very powerful tool in the theory of random matrices.

Definition 2.11. The Resolvent.

Let $T : D(T) \rightarrow X$ with $D(T) \subseteq X$ be a linear bound operator on a Banach space X .

Let $\sigma(T)$ be the spectrum of T and $\rho(T) := \mathbb{C} \setminus \sigma(T)$ be the resolvent set. Then the resolvent mapping

$$\rho(T) \ni z \mapsto R_z(T) := (T - z \cdot \text{id})^{-1}$$

maps to the resolvent of T for $z \in \rho(T)$.

During eigenvalue approximation and evaluation of correlators we will discuss fourier transformed random variables, for which we now clarify their definition by introducing the *Fourier transformation*.

Definition 2.12. Fourier Transformation.

Let $f \in \mathcal{L}^1(\mathbb{R}^d)$ be a λ integrable function. Then we define the *Fourier transformation* $\mathcal{F} : \mathcal{L}^1(\mathbb{R}^d) \rightarrow C_0(\mathbb{R}^d)$ by

$$(\mathcal{F}f)(\xi) := \int_{\mathbb{R}^d} f(x) \cdot e^{i \cdot \langle x, \xi \rangle} \lambda(dx).$$

The *inverse Fourier transformation* is then only defined for $f \in \mathcal{S}(\mathbb{R}^d)$ by $(\mathcal{F}^{-1}g)(x) := \int_{\mathbb{R}^d} g(\xi) \cdot e^{-i \cdot \langle x, \xi \rangle} \lambda(d\xi)$. We denote $\bar{\lambda} := (2\pi)^{-d} \cdot \lambda$ and $\hat{f} := \mathcal{F}f$.

Note that within our definition we pushed the normalization factor $(2\pi)^{-d}$ to the inverse Fourier transform, which is a common practice in the literature [3] and motivated by convenience. The first important Fourier transformation we will discuss is the one of the Dirac distribution.

Corollary 2.1. Fourier Transformation of Delta Distributions.

Let $y \in \mathbb{R}^d$ be a fixed point and $\mathcal{S}'(\mathbb{R}^d) \ni \delta_y : \varphi \mapsto \varphi(y)$ be the Dirac delta distribution at y . Then the Fourier transform of δ_y is given by

$$(\mathcal{F}\delta_y)(\varphi) = [e_y](\varphi) := \int_{\mathbb{R}^d} \exp(i \cdot y \cdot x) \cdot \varphi(x) \lambda(dx).$$

Proof. Since δ_y for $y \in \mathbb{R}^d$ is an element of $\mathcal{S}'(\mathbb{R}^d)$ we can evaluate for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ the Fourier transform of δ_y as

$$(\mathcal{F}\delta_y)(\varphi) = \delta_y(\mathcal{F}\varphi) = (\mathcal{F}\varphi)(y) = \int_{\mathbb{R}^d} \varphi(x) \cdot \exp(i \cdot y \cdot x) \lambda(dx),$$

which is exactly our claimed result. q.e.d.

The interpretation of this statement is much simpler than its formulation might seem, since it suggests that $(\mathcal{F}\delta_y)(x) = \exp(i \cdot x \cdot y)$, which is exactly the kernel of said integral. This will be of use later on when we discuss the probability density correction of the critical equilibrium positions.

Lastly to gain the Green's function that will state the bare propagator, we will make use of the *Laplace transformation* when facing a differential equation in random variables.

Theorem and Definition 2.1. Laplace Transformation.

Let $f : \mathbb{R}_{\geq 0} \rightarrow \mathbb{C}$ be a function of *exponential order*, i.e. $\exists C, s_0, T \in \mathbb{R}_{>0}$ with $|f(t)| \leq C \cdot e^{s_0 \cdot t}$ for $t \geq T$ and let $t \mapsto |f(t)|$ be λ -integrable on $[0, T]$, i.e. $\int_{[0, T]} |f(t)| \lambda(dt) < \infty$. Then there exists the Integral

$$(\mathcal{L}f)(s) := \int_{\mathbb{R}_{\geq 0}} f(t) \cdot e^{-s \cdot t} \lambda(dt)$$

for all $s \in \mathbb{C}$ with $\operatorname{Re}(s) > s_0$. We then call $(\mathcal{L}f)(s)$ the *Laplace transformation* of f .

Before we start to develop the physical and mathematical theory of ERM, a remark to general notation. We will use the following symbols throughout the thesis:

| Symbol | Meaning |
|--|---|
| \circ | Composition of functions |
| $\langle v, w \rangle$ | Scalar product of vectors v, w |
| $\ v\ $ | Norm of vector v |
| \mathbb{E} | Expectation value |
| \mathbb{E}_r | Expectation value with respect to r |
| \mathbb{P} | Probability measure |
| $\langle \cdot \rangle_{\mathbb{P}}$ | Expectation value with respect to \mathbb{P} |
| $\langle \cdot \rangle_{\mathbb{P}(dr)}$ | Expectation value with respect to $\mathbb{P}(dr)$ |
| M^\perp | Transposed matrix of $M \in K^{n \times m}$, K a field |
| $B_r(x) \subset V$ | for $r > 0$ Ball in $(V, \ \cdot\)$ defined by $\{v \in V : \ v - x\ < r\}$ |
| $\partial B_r(x)$ | Boundary of $B_r(x)$ def. by $\{v \in V : \ v - x\ = r\}$ |
| $B_{r,R}(x)$ | for $r < R$ Annulus def. by $B_R(x) \setminus B_r(x)$ |

2.2 Foundations

Having established this basic mathematical framework, we can now move on to describing the *physics* of our system. The ERM model stated in [3, 4, 8, 9] and other is used to describe a classical physical system of $N \in \mathbb{N}$ interacting particles in a d -dimensional space. A visualization was done in the chapter's introduction, see figure 1. This space where the particles individually are *located* is from now on referred to as $\Gamma \subset \mathbb{R}^d$ with some technical assumptions on its structure. A summary of all particles positions is encoded in the *phase space* $V_{d,N}$ which is given by the cartesian product of N copies of Γ .

Definition 2.13. Modelling Space.

We call an \mathbb{R}^d -open, relatively compact subspace $\Gamma \subset \mathbb{R}^d$ for $d \in \mathbb{N}$ the *modelling space* of the particles. We then understand $V_{d,N} := \Gamma^N$ to be the *phase space*.^a

^aImplicitly we also define for technicality an isomorphism $\iota : (\mathbb{R}^d)^N \rightarrow \mathbb{R}^{d \cdot N}$ by $\iota(v) = (v_{1,1}, \dots, v_{1,d}, \dots, v_{N,1}, \dots, v_{N,d})$. To not overcomplicate the notation we will not further distinguish between $(\mathbb{R}^d)^N$ and $\mathbb{R}^{d \cdot N}$.

Our general idea now is to assume an at least three times (see T.2.1) continuously differentiable potential function $U : V_{d,N} \rightarrow \mathbb{R}$ describing the system state, i.e. the potential energy of $N \in \mathbb{N}$ particles numbered $i \in [N]$ placed at positions $r_i \in \Gamma$. For later purposes of approximation we would now like to only consider positional arguments which fulfill U -critical conditions, i.e. physically speaking *equilibrium* states of the system. These also do exist for U since we made according assumptions on $\Gamma \subset \mathbb{R}^d$.

Definition 2.14. Critical Distribution of Positions.

We call $r_* \in V_{d,N}$ a critical distribution of positions with respect to U if $dU(r_*) = 0$. We denote such to be in $\text{critP}(U)$.

From this mathematical definition we can already deduce physical properties, since being in a critical state physically means that *movement* is (even instably) *restricted*. One could now wonder what happens if we dislocate the particles from their equilibrium positions ever so slightly. Intuitively, if we have an unstable equilibrium, i.e. mathematically a saddle point, we would expect the particles to move to lower states of potential energy, i.e. minima of U . But even in stable equilibria, our physical intuition expects a *restoring force* to act on the particles, which would bring them back to their equilibrium positions. Mathematically we can analyse this behaviour by looking at the first orders of the *Taylor series* of U . But if we want our positions to be and remain within a restricted volume $\Gamma \subseteq \mathbb{R}^d$, we need to first artificially restrict allowed variations of $r_* \in \text{critP}(U)$ to *Taylor fluctuations*, i.e. elements of $\text{TF}(\Gamma, r_*)$.

Definition 2.15. Taylorfluctuations.

Let $r \in V_{d,N}$, then we define $\phi \in (\mathbb{R}^d)^N$ as *Taylorfluctuation* around r , if^a $\phi_i \in B_{\text{dist}(r_i, \Gamma)}(0_{\mathbb{R}^n})$ for $i \in [N]$. We denote such to be in $\text{TF}(\Gamma, r)$.

^aWe denote $\text{dist}(r_i, \Gamma) := \inf_{x \in \partial\Gamma} (\|x - r_i\|_2)$ as the minimal distance from any point r_i to the boundary of Γ .

Since for Taylor approximation from theorem 2.1 we assume our displacement to be small for the remaining summand $R_{p+1}(f, r_*, h)$ to be equally small, we always find allowed $\phi \in \text{TF}(\Gamma, r_*)$ for any $r_* \in \text{critP}(U)$ because of the openness of Γ . If we perform a large volume limit on $V_{d,N}$, we will be able to neglect the restriction to $\text{TF}(\Gamma, r_*)$ and consider all of \mathbb{R}^d as our displacement space. Another approach is a global shift of the modelling space's origin to r_* , by which the Taylor fluctuations can be drawn from a constant set $\text{TF}_{\Gamma,0} =: \text{TF}_{\Gamma,N}$, which can be pictured as shown in figure 2.

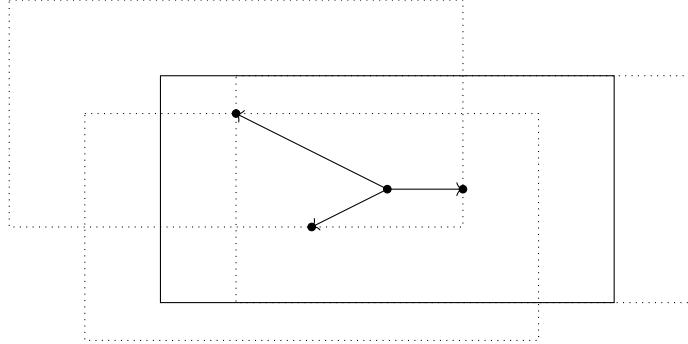


Figure 2: Mapping of $\text{critP}(U)$ to Γ_2 in the ERM model.

Within the ERM model we are not interested in the particles moments, such that the hamiltonian of the system is fully given by the potential energy U .

Definition 2.16. The Hamiltonian.

Let $U \in C^2(V_{d,N})$ for $\Gamma \subset \mathbb{R}^d$ and $V_{d,N} := \Gamma^N$ be a potential energy function of a system of $N \in \mathbb{N}$ particles. For $r \in V_{d,N}$ and $\phi \in \text{TF}(V_{d,N}, r)$ we define the corresponding $H(r, \phi) := U(r + \phi)$. Its approximation will be denoted by $H^{(n)}(r, \phi) := \sum_{k=0}^n \frac{1}{k!} D_\phi^k U(r)^k$.

^aWe denote the differential operator D_ϕ^k as the k -th derivative of U with respect to its argument r in direction ϕ . At first order we therefore have $D_\phi U(r) = \frac{d}{dt} U(r + t\phi)|_{t=0}$.

The Potential U (now equivalent to its hamiltonian H) can now be approximated at $r_* \in \text{critP}(U)$ to second order with displacement $\phi \in \text{TF}(V_{d,N}, r_*)$ by

$$H^{(2)}(r_*, \phi) = U(r_*) + \underbrace{\frac{d}{dt} U(r_* + t \cdot \phi)|_{t=0}}_{=0} + \frac{1}{2} \cdot \langle HU(r_*) \cdot \phi, \phi \rangle,$$

where $HU(r_*)$ denotes the hessian of U at r_* . This now as initially stated gives an integral of the form

$$\int_{V_{d,N}} \int_{\text{TF}(V_{d,N}, r_*)} \exp(-\beta \cdot U(r_*)) \cdot \exp\left(-\beta \cdot \frac{1}{2} \cdot \langle HU(r_*) \cdot \phi, \phi \rangle\right) \lambda(d\phi) \lambda(dr_*).$$

Within the following pages representing the current standpoint of research one assumed $\exp(-\beta \cdot U(r_*))$ to be constantly given by the a priori density $1/|V_{d,N}|$ with $|V_{d,N}| := \lambda(V_{d,N})$ and therefore of no greater interest. With $\text{TF}(V_{d,N}, r_*)$ also assumed to be *independent*² of r_* (see above), such that it is set to a fixed set $\text{TF}_{\Gamma,N} \subset (\mathbb{R}^d)^N$. This shifted the startpoint from $\int 1 \mathbb{P}$ effectively approximating to

$$\begin{aligned} & \int_{V_{d,N}} \int_{\text{TF}(V_{d,N}, r_*)} \exp\left(-\beta \cdot \frac{1}{2} \cdot \langle HU(r) \cdot \phi, \phi \rangle\right) \lambda(d\phi) \left(\frac{1}{|V_{d,N}|} \cdot \lambda\right)(dr) \\ & \approx \int_{V_{d,N} \times \text{TF}_{\Gamma,N}} \underbrace{\frac{1}{|V_{d,N}|} \cdot \exp\left(-\frac{\beta}{2} \cdot \langle HU(r) \cdot \phi, \phi \rangle\right)}_{= \exp(-\beta \cdot H_*(r, \phi))} \lambda(d(r_*, \phi)), \end{aligned}$$

defining an a priori Hamiltonian H_* , in which the distribution of the shifting vector ϕ is now much more prominent. With growing progress in this thesis investigation it will become clear that the original exponential term is indeed of interest, which will lead to a corrected hamiltonian H . But first we need to discuss current integrand at hand. A regard to notation: In referenced literature these two integrals are noted using two different symbols. For averaging over the critical position domain it is established to use an overline “—”, while for the translational domain of ϕ the symbol “⟨...⟩” is used, see for example [3, 4].

We now need to motivate the use and definition of ERM for our system. This can be done by assuming *pair interactions* between the particles. This is a common assumption in physics, since it is often the case that particle potentials can be written as a sum of pair potentials. Therefore with $r \in V_{d,N}$ we have the representation

$$U(r) = \frac{1}{2} \cdot \sum_{i,j \in [N]} U(r_i - r_j).$$

Performing two differentiations on U with respect to r we get for $[N]^2 \ni (i, j) \mapsto d_{i,j} : r \mapsto r_i - r_j$ the form $(\frac{d}{dr})^2(U \circ d_{i,j}) = U''(d_{i,j}) \cdot d'_{i,j}^2 + U'(d_{i,j}) \cdot d''_{i,j}$. For $d'_{i,j}(r) = e_i + e_j$ and $d''_{i,j}(r) = 0$ we find using $d'_{i,j}(r)^\top \cdot g'_{i,j}(r) = 2$ the second derivative as

$$U''(r) = \frac{1}{2} \cdot \sum_{(i,j) \in [N]^2} \left(\frac{d}{dr}\right)^2 (U \circ d_{i,j}) = \frac{1}{2} \cdot 2 \cdot \sum_{i,j \in [N]} U''(r_i - r_j). \quad (1)$$

This physically represents exactly the idea of a feathered potential, since for an energy $E(x) = k \cdot x^2/2$ we have $E''(x) = k$. Therefore we can treat U'' as a spring function that yields a k dependent on the distance of two particles. If we now neglect the directions, i.e. making U''

²The error made by this assumption is not to be discussed in this thesis.

a radial function, we can implement a pair interaction function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ that is a radial function and constitutes the hessian of U with the following properties.

Definition 2.17. Pair Interaction Function (PIF).

We call $f \in \mathcal{S}(\mathbb{R}^d)$ a *pair interaction function* if $\exists f_{||} \in \mathbb{R} \rightarrow \mathbb{R}$ such that $f = f_{||} \circ \|\cdot\|_2$, i.e. f is radially symmetric, and $f \geq 0$. Furthermore for $x \in \partial B_r(0)$ with $r \rightarrow \infty$ we require $f(x) = 0$. We denote such functions to be in $Spr(\mathbb{R}^d)$.

Physically speaking, by introducing a radial symmetry with $f = f_{||} \circ \|\cdot\|_2$, we want the particles to interact equally with each other without any preference of direction. The second condition of f being a Schwartz function is a technical condition to ensure fourier transformability. Comparing results to $H^{(2)}$ now gives us

$$H(r_0, \phi) \approx \frac{1}{2} \cdot \sum_{i,j \in [N]} U(r_i - r_j) + \frac{1}{4} \cdot \sum_{i,j \in [N]} f_{||}(\|r_i - r_j\|_2) \cdot \phi_i \cdot \phi_j,$$

with $r_0 \in \text{critP}(U)$ and $\phi \in \text{TF}(V_{d,N}, r_0)$. This is also a good moment to discuss units in our model. It would be natural to assume r having the units of length, i.e. m, as well as ϕ which is directly added to r . But since a mathematical theory of units and dimensional analysis is way beyond the scope³ of this thesis, we will assume all occurring physical quantities to be dimensionless, which can be achieved by multiplication with a normalized inverse quantity. In practice this means $r = r \cdot \sigma_m^{-1}$ as well as $\phi = \phi \cdot \sigma_m^{-1}$ and therefore $[r] = 1 = [\phi] = [U] = [G]$ [4].

Having introduced the pair interaction function f we can now take a look at our aimed approximation of the hessian of U at $r_* \in \text{critP}(U)$. The core of the repulsive ERM theory given in [3, 4] is a *laplacian* matrix $L \in \mathbb{R}^{N \times N}$, which is strongly related to graph theory. Without going too much into detail, using D.2.4 the decomposition $L = B \cdot B^\top = D - W$ with B being the incidence matrix (see D.2.5), D the degree matrix (see D.2.2) and W the weighted adjacency matrix (see D.2.3) of a graph (see D.2.1) can be stated [6]. The first matrix B encodes the *bonds* between the particles as their signed square roots $\pm \sqrt{L_{i,j}}$, respectively for *incoming* and *outgoing* edges. This matrix will be holding the pair interaction function as $\pm \sqrt{f}$ in its entries. From it we can deduce $\langle L \cdot x, x \rangle = \langle B^\top x, B^\top x \rangle = \|B^\top \cdot x\|_2^2 \geq 0$ with B symmetric for all $x \in \mathbb{R}^{d \cdot N}$, which is the property of positive semi-definiteness. The second property⁴ $i \mapsto \sum_{j \in [d \cdot N]} L_{i,j} = 0$, i.e. the rows of L summing up to zero, translates into $1_{\mathbb{R}^{d \cdot N}} = (1, \dots, 1)$ being an eigenvector to the eigenvalue 0.

This directly corresponds to the physical picture: The nodes of the graph are the particles, the edges are the interactions between them and the weights define the strength of the interaction.

The euclidean part in ERM comes from the constraint of our target space $V_{d,N}$ having euclidean structure, which is straightforwardly given by the relation $V_{d,N} \subseteq \mathbb{R}^{d \cdot N}$ and the induced euclidean norm⁵ $\|\cdot\|_2 := \sqrt{\langle \cdot, \cdot \rangle}$ that is already part of Definition 2.17. This intuitively

³See for example the *Buckingham π theorem*, the paper *Dimensioned Algebra: the mathematics of physical quantities* by Carlos Zapata-Carratala or others.

⁴Sometimes one writes $\sum_{i \sim j}$ for nodes (v_1, \dots, v_N) . This means summing only over all *adjacent* nodes. Because in our system every particle interacts with every other particle, we can write $\sum_{j \in [N]}$ instead.

⁵The norm can indeed be freely chosen since we have an equivalence theorem for all p norms build by

corresponds to our physical understanding of three dimensional space. With this we can now introduce the heart of the ERM model, the laplacian matrix $\tilde{U}(f, r_*)$.

Postulate 2.1. Coupling Representation.

Let $U \in C^3((\mathbb{R}^d)^N)$ describe the pair potential function. For^a $(i, j) \mapsto f_{i,j} = U'' \circ g_{i,j}$ it holds^b $\langle HU(r) \cdot \phi, \phi \rangle = \langle \tilde{U}(f, r) \cdot \phi, \phi \rangle$ for $r \in V_{d,N}$ and $\phi \in \text{TF}(\Gamma, r)$ with $\tilde{U}(f, r)$ having the general form

$$\tilde{U}(f, r_*) := \begin{pmatrix} \Sigma(f, 1) \cdot I_d & -\tilde{f}_{1,2} \cdot I_d & \cdots & -\tilde{f}_{1,N} \cdot I_d \\ -\tilde{f}_{2,1} \cdot I_d & \Sigma(f, 2) \cdot I_d & \cdots & -\tilde{f}_{2,N} \cdot I_d \\ \vdots & \vdots & \ddots & \vdots \\ -\tilde{f}_{N,1} \cdot I_d & -\tilde{f}_{N,2} \cdot I_d & \cdots & \Sigma(f, N) \cdot I_d \end{pmatrix} \in \mathbb{R}^{d \cdot N \times d \cdot N}$$

We denoted $f_{i,j} := f(r_i - r_j)$ for $i, j \in [N]^2$ and $\Sigma(f, i) := \sum_{j \in [N] \setminus \{i\}} f_{i,j}$.

^aAs in $d_{i,j}(r) := r_i - r_j$ stating the difference vector of r_i and r_j following equation (1).

^bTechnically speaking for multiplication we need to use an isomorphism $(\mathbb{R}^d)^N \rightarrow \mathbb{R}^{d \cdot N}$ to make the matrix multiplication work. For this we propose a projection π of the form $((., ., ., .), \dots) \mapsto (., ., ., ., \dots)$. Then we would have $\langle HU(r_*) \cdot \phi, \phi \rangle = \langle \tilde{U}(f, r) \cdot \pi(\phi), \pi(\phi) \rangle$.

Note that if we would introduce the PIF f with the property $f(0) = 0$ we can simply take the sum over all matrix columns, i.e. $\sum_{j \in [N]} f_{i,j}$. Because $\tilde{U}(f, r_*)$ is constructed of block matrices, we physically only use the norm of ϕ , i.e. only its *length*, not its *direction*. This is a reduction of complexity, as the matrix in general holds non-diagonal blocks. Therefore a smaller matrix $M(f, r_*)$ can be defined as $M(f, r_*)_{i,j}$ being the diagonal entry of the i, j -th block of $\tilde{U}(f, r_*)$. We do not notationally differentiate the matrix $\tilde{U}(f, r_*) \in \mathbb{R}^{N \times N}$ where $\tilde{U}(f, r_*)_{i,j}$ is the diagonal entry of the i, j -th block from the general matrix $\tilde{U}(f, r_*) \in \mathbb{R}^{d \cdot N \times d \cdot N}$.

To introduce the randomness in euclidean *random* matrices we now only need to exchange the fixed positions $r_* \in V_{d,N}$ by random variables coming from an abstract probability space $(\Omega, \Sigma, \mathbb{P})$ mapping to $(V_{d,N}, \mathcal{B}(V_{d,N}))$. This makes our matrix representation also random, i.e. $\Omega \ni \omega \mapsto \tilde{U}(f, R_\omega)$ becoming a *random matrix*, where $R : \Omega \rightarrow V_{d,N}$ is said random variable of positions. Doing so we find for every $\omega \in \Omega$ a initial distribution of positions in our space Γ , on which we later can calculate the expectancy via the pushforwad measure $\mathbb{P}_R := \mathbb{P} \circ R^{-1}$.

Definition 2.18. Position Distribution.

Let $(\Omega, \mathcal{A}, \mathbb{P})$ be a probability space and $V_{d,N}$ a position space. A *position distribution* then is a random variable $X : \Omega \rightarrow V_{d,N}$ for $N \in \mathbb{N}$ particles.

2.3 Eigenvalue Measurement

$\|x\|_p := \left(\sum_{i \in [d]} |x_i|^p \right)^{1/p}$ for $p \in \mathbb{N}$ and $x \in \mathbb{R}^d$.

The general interest now lies in exploring the eigenvalue measurement, i.e. the measurement of the eigenvalue density of $\tilde{U}(f, R_\omega)$ for $\omega \in \Omega$. To do so we first need to discuss general approaches and then stick to one particular method which will come in handy from a perturbative perspective.

Beginning with a general insight we should imagine fixed eigenvalues in the point spectrum of $\sigma_p(\tilde{U}(f, R_\omega)) \subset \mathbb{C}$ with finite cardinality $m := \#\sigma_p(\tilde{U}(f, R_\omega))$ that we can count bijectively via $\Lambda : [m] \rightarrow \sigma_p(\tilde{U}(f, R_\omega))$. We now want to *test for* those eigenvalues, i.e. we choose a testpoint $P \in \mathbb{C}$ or even set $\mathcal{P} \subseteq \mathbb{C}$ to compare with the set of eigenvalues $\sigma_p(\tilde{U}(f, R_\omega))$. Testing positive should return us a 1, testing negative a 0. This can be done by the use of *dirac* measures $i \mapsto \delta_{\Lambda_i}(\{P\})$ for every single eigenvalue Λ_i of the considered matrix. It makes sense now to sum up all the results of $\delta_{\Lambda_i}(\{P\})$ to gain the total successes for the testpoint P and normalizing by the total number of eigenvalues m to get the *probability of success* for the testpoint P . This measure is known in literature [10] as the *empirical spectral measure*. In a last step the averaging over all possible euclidean random matrices given by $\Omega \ni \omega \mapsto U(f, R_\omega)$ for a fixed particle position random variable $R : \Omega \rightarrow V_{d,N}$ can now be done via integration, such that we get $g_{\tilde{U}(f, R)}$ as

$$g_{\tilde{U}(f, R)}(P) = \frac{1}{p} \cdot \int_{\Omega} \underbrace{\sum_{i \in [p]} \delta_{\Lambda(\omega)_i}(\{P\})}_{=: I_P(\omega)} \mathbb{P}(d\omega) = \frac{1}{p} \cdot \sum_{I_* \in \text{im}(I_P)} I_* \cdot \mathbb{P}(\{I_P = I_*\}). \quad (2)$$

We have tacitly used a notation from measure theory declared by $\{I_P = I_*\} := \{\omega \in \Omega : I_P(\omega) = I_*\}$ and an implicitly defined function $\Lambda : \Omega \ni \omega \mapsto ([m] \rightarrow \sigma_p(\tilde{U}(f, R_\omega)))$. Since we can already notice by just writing down the hard time we have to correctly handle this object, we try to use complex analysis to approximate our idea. The strategy can be neatly presented in a visualization, see figure 3:

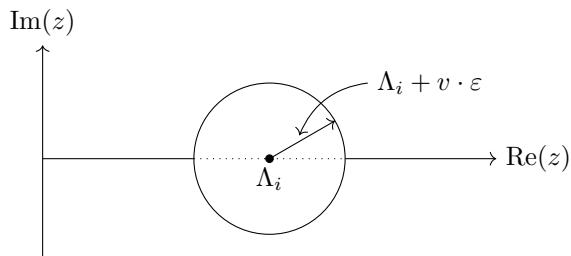


Figure 3: Approximation of eigenvalues Λ_i by a complex number $z = \Lambda_i + v \cdot \varepsilon$ for a direction $v \in B_\varepsilon(0) \subset \mathbb{C}$. The easiest choice of direction is $v = \vec{i}$, since all $\Lambda_i \in \mathbb{R}_{\geq 0}$ for our positive semidefinite laplacian matrix. With $\varepsilon > 0$ we can get arbitrarily close to the eigenvalue Λ_i .

To utilize this technically we make use of the resolvent in definition 2.11 regarding $\tilde{U}(f, R_\omega)$, which for eigenvalues $i \mapsto \Lambda_i$ can be brought to a divergent pole. But first we want to motivate this idea from a physical perspective.

The intuition for the resolvents appearance lies in the newtonian dynamics on which our system relies. If we, in a more general case, allow statistical processes such as $X : \mathbb{R}_{>0} \rightarrow$

$(\Omega \rightarrow V_{d,N})$ with sufficient requirements⁶, then for two particles their interaction is given by the weights within the entries of our Laplace matrix $\tilde{U}(f, X_t)$ for any time $t \in \mathbb{R}_{>0}$. Because of their symmetry we can write the force acting on particle $X_t(\omega)_i$ caused by particle $X_t(\omega)_j$ at time t as

$$\left(\frac{d}{dt}\right)^2 X_t(\omega)_i = -\tilde{U}(f, X_t(\omega))_{i,j} \cdot X_t(\omega)_j.$$

We can now transfer this statistical ordinary differential equation to the initial state of the impacted particles displacement $X_t(\omega)_i$ at different points in time as

$$\left(\frac{d}{dt}\right)^2 \langle X_t(\omega)_i, X_0(\omega)_i \rangle = -\tilde{U}(f, X_t(\omega))_{i,j} \cdot \langle X_t(\omega)_j, X_0(\omega)_i \rangle.$$

Application of the Laplace transformation from Theorem and Definition 2.1 under appropriate conditions yields

$$\begin{aligned} \int_{\mathbb{R}_{>0}} \left(\frac{d}{dt}\right)^2 \langle X_t(\omega)_i, X_0(\omega)_i \rangle \cdot \exp(-s \cdot t) \lambda(dt) \\ = -\tilde{U}(f, X_t(\omega))_{i,j} \cdot \int_{\mathbb{R}_{>0}} \langle X_t(\omega)_j, X_0(\omega)_i \rangle \cdot \exp(-s \cdot t) \lambda(dt). \end{aligned}$$

Let $F_{j,i,\omega}(t) := \langle X_t(\omega)_j, X_0(\omega)_i \rangle$ for now. For derivatives under Laplace transformations we can utilize Lemma 1, which is proven in the appendix.

Lemma 1 (Laplace Transformation of n -th Derivatives). Let $f \in C^n(\mathbb{R}_{>0})$ be of exponential order for $C, s_0, T > 0$. Then for $n \in \mathbb{N}$ we have

$$(\mathcal{L}f^{(n)})(s) = s^n \cdot (\mathcal{L}f)(s) - \sum_{k=0}^{n-1} s^{n-1-k} \cdot f^{(k)}(0).$$

With it we find $\int_{\mathbb{R}_{>0}} \frac{d}{dt} f(t) \cdot \exp(-s \cdot t) \lambda(dt) = -f(0) + s \cdot (\mathcal{L}f)(s)$ that can be used for $t \mapsto F''_{j,i,\omega}(t)$ to yield

$$\int_{\mathbb{R}_{>0}} \left(\frac{d}{dt}\right)^2 F_{i,i,\omega}(t) \cdot \exp(-s \cdot t) \lambda(dt) = -\frac{d}{dt} F_{i,i,\omega}(0) - s \cdot F_{i,i,\omega}(0) + s^2 \cdot (\mathcal{L}F_{i,i,\omega})(s).$$

This introduces two initial conditions, the initial displacement and initial velocity, that can be set using physical reasoning that we will discuss in a moment. If we first introduce artificially $\delta_{ij} := \mathbb{1}_{\{i\}}(j)$ we can rearrange terms using the equality to $-\tilde{U}(f, X_t(\omega)) \cdot (\mathcal{L}F_{j,i,\omega})(s)$ to isolate the initial conditions:

$$(s^2 \cdot \delta_{ij} + \tilde{U}(f, X_t(\omega))) \cdot (\mathcal{L}F_{j,i,\omega})(s) = F_{j,i,\omega}(0) + s \cdot \frac{d}{dt} F_{j,i,\omega}(0).$$

To choose these initial values reasonably, we argue that particles only correlate with each other, i.e. defining $F_{j,i,\omega}(0) = \delta_{ij}$, and the correlation of ones particle velocity at $t \rightarrow 0$ with the

⁶See L.1 and TD.2.1. Explicitly for the existence of the Laplace transform, several requirements need to be met by $t \mapsto \langle X_t(\omega), X_0(\omega) \rangle$. Since in this thesis the actual *time dependent process* is not of interest, i.e. only a discussion of a frozen system is done, we do not specify this further.

starting position of another particle is zero, i.e. $\frac{d}{dt}F_{j,i,\omega}(0) = 0$. This means that the systems dynamics are *caused by* the initial systems state with development of time t and not hard-wired into the initial conditions at $t = 0$. Setting $s = \overset{\circ}{i} \cdot \Lambda_i$ with $\Lambda_i > s_0 > 0$ we can reformulate to

$$(\mathcal{L}F_{j,i,\omega})(s) = \frac{1}{s^2 \cdot \delta_{ij} + \tilde{U}(f, X_t(\omega))_{i,j}} \stackrel{\varepsilon \rightarrow 0}{=} \frac{1}{\tilde{U}(f, X_t(\omega))_{i,j} - \delta_{ij} \cdot \Lambda_i^2}.$$

and interpret $(i, j) \mapsto F_{j,i,\omega}(s)$ as the resolvent $(\tilde{U}(f, X_t(\omega)) - \text{diag}(\Lambda_i^2))^{-1}$ of the Laplace matrix $\tilde{U}(f, X_t(\omega))$. An implicit discrete Fourier transformation of the resolvents components $F_{j,i,\omega}(s)$ can be done by the summation

$$(p, s) \mapsto \sum_{(i,j) \in [d:N]^2} \frac{1}{\tilde{U}(f, X_t(\omega))_{i,j} - \delta_{ij} \cdot \Lambda_i^2} \cdot \exp(\overset{\circ}{i} \cdot \langle p, r_{\tau(i)} - r_{\tau(j)} \rangle).$$

In his we have introduced a mapping τ which treats dimensionality issues and collects the matching particle positions for subtraction. It therefore needs a form $[N \cdot d] \rightarrow [N]^d$. We again do not discuss this further. Instead we summarize the result in the following postulate.

Postulate 2.2. Eigenvalue Density via the Resolvent.

Let $M \in \mathbb{R}^{d \cdot N \cdot d \cdot N}$ and $\rho(M)$ the resolvent set of M . Then for $z \in \rho(M)$ we measure the eigenvalue density via the expectancy of the discretely Fourier transformed resolvent

$$G_N(p, z) := \int_{\Omega} \sum_{(i,j)} R_z(M)_{i,j} \cdot e^{\overset{\circ}{i} \cdot \langle p, R_{\tau(i)} - R_{\tau(j)} \rangle} \mathbb{P}(d\omega),$$

where τ is a mapping of technical nature.

The only missing connection to be made is the one between the resolvent and the empirical spectral measure. It is made using the residual theorem from complex analysis, meaning

$$g_{\tilde{U}(f,R)}(P) = \frac{1}{\overset{\circ}{i} \cdot \pi} \cdot \frac{1}{N} \cdot \sum_{j=1}^N \frac{1}{\Lambda_j - \underbrace{(\Lambda_j + \overset{\circ}{i} \cdot \varepsilon)}_{=: z_j(\varepsilon)}} = \frac{1}{\overset{\circ}{i} \cdot \pi} \cdot \frac{1}{N} \cdot \sum_{j=1}^N \left[\frac{1}{\text{diag}(\Lambda) - \text{diag}(i \mapsto z_i(\varepsilon))} \right]_{j,j}.$$

The sum can now be expanded onto $[N]^2$ using δ_{ij} and its approximation on using an exponential limit $\lim_{||p|| \rightarrow \infty} \exp(\overset{\circ}{i} \cdot \langle p, r_{\tau(i)} - r_{\tau(j)} \rangle)$ known as a *large momentum limit*. But since this connection is not of particular use for the further development of the thesis, we only state

$$g(s) = -\frac{1}{\pi} \cdot \lim_{||p|| \rightarrow \infty} \left(\text{Im} \left(\lim_{\varepsilon \rightarrow 0} G_N(p, s^2 + \overset{\circ}{i} \cdot \varepsilon) \right) \right),$$

The procedure can be seen in [11].

To introduce the perturbative machinery we use a gaussian approach to the resolvent. Hereby we use the second moment of a gaussian probability measure that is connected to the resolvent. This is done in the following postulate.

Postulate 2.3. Resolvent Representation via second Moment.

For $\Omega \ni \omega \mapsto \tilde{U}(f, R_\omega)_{i,j}$ normally distributed with expectancy $\mu_{i,j} = 0$ and correlation matrix $R_z(\tilde{U}(f, R_\omega))$ as the resolvent of $\tilde{U}(f, R_\omega)$, there exists a gaussian density $\mathcal{G}_{R_z(\tilde{U}(f, R_\omega))} : \mathbb{R}^{3 \cdot N} \rightarrow \mathbb{R}$ according to Definition 2.9 such that

$$(z - \tilde{U}(f, R_\omega))_{i,j}^{-1} = \frac{1}{I_{\tilde{U}(f, R_\omega)}(z)} \cdot \int_{\mathbb{R}^{d \cdot N}} \phi_i \cdot \phi_j (\mathbb{G}_{\tilde{U}, z, R_\omega})(d\phi).$$

Within we introduced a gaussian measure $\mathbb{G}_{\tilde{U}, z, R_\omega}$ representing $\mathcal{G}_{R_z(\tilde{U}(f, R_\omega))} \cdot \lambda$ and $I_{\tilde{U}(f, R_\omega)}(z) := \int_{\mathbb{R}^{3 \cdot N}} 1 (\mathcal{G}_{R_z(\tilde{U}(f, R_\omega))} \cdot \lambda) \in \mathbb{R}$ for normalisation.

Notice how we have introduced this postulate using $-(z - \tilde{U}(f, R_\omega))$. We choose to do so to follow literature's convention [4]. The resolvent we have derived would lead to a completely analogous result. This postulate leads to a different form of G_N , i.e. the expectancy in $\omega \in \Omega$ of

$$\sum_{(i,j) \in [d \cdot N]^2} \exp(\hat{i} \cdot \langle p, R_{\omega \tau(i)} - (R_\omega)_{\tau(j)} \rangle) \cdot \frac{1}{I_{\tilde{U}(f, R_\omega)}(z)} \cdot \int_{\mathbb{R}^{d \cdot N}} \phi_i \cdot \phi_j (\mathbb{G}_{\tilde{U}, z, R_\omega})(d\phi).$$

In perturbation theory we now need to assign the role of an action functional to some component of said integral. As we have established in Postulate 2.3 the resolvent can be written as a second moment of a gaussian probability measure $\mathbb{G}_{\tilde{U}, z, R_\omega}$, which introduces a gaussian density function $\mathcal{G}_{\tilde{U}(f, R_\omega)}$ of the form

$$\mathcal{G}_{R_z(\tilde{U}(f, R_\omega))}(\phi) = \frac{1}{\sqrt{(2 \cdot \pi)^{d \cdot N} \cdot \det(R_z(\tilde{U}(f, R_\omega)))}} \cdot \exp\left(-\frac{1}{2} \cdot \underbrace{\langle \phi, (z - \tilde{U}(f, R_\omega)) \cdot \phi \rangle}_{=: S_{z, R_\omega}(\phi)}\right). \quad (3)$$

Within the exponent we can identify the *action function* $S_{z, R_\omega} : \mathbb{R}^{d \cdot N} \rightarrow \mathbb{R}$ that is the starting point going forward.

Definition 2.19. Discrete Action.

Let $z \in \mathbb{C}$ and $R : (\Omega \rightarrow V_{d,N})$, then for $\tilde{U}(f, R_\omega)$ we define $S_{z, R_\omega}(\phi) := \langle (\tilde{U}(f, R_\omega) - z) \cdot \phi, \phi \rangle$ as the *discrete action* of the ERM model.

The tricky part now involves a well reasoned transition from a discrete *function of vectors* S_{z, R_ω} to a *functional of functions* $S_{z, R_\omega} : \mathcal{F}_{d,N} \rightarrow \mathbb{R}$. Note that we do not change notation for the action functional, since its physical interpretation remains the same. To create such a functional we expand the scalar product notation of $S_{z, R_\omega} : \mathbb{R}^{d \cdot N} \rightarrow \mathbb{R}$ to its summation form

$$S_{z, R_\omega}(\phi) = \sum_{(i,j) \in [d \cdot N]^2} \phi_i \cdot (z - \tilde{U}(f, R_\omega))_{i,j} \cdot \phi_j. \quad (4)$$

We now introduce a trick constituted of two parts. First we extrapolate the variables ϕ_i to a

general Schwartz function⁷ $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ which fits the restriction of $\Phi(x) = \phi_i$ for equilibrium position arguments $x = R_\omega(\tau^{-1}(i))$. This means that Φ yields not closer defined values at non equilibrium positions, which in the second step should be eliminated by a Dirac integration, since they do not appear in our original discrete action. Plugging this into the discrete action yields⁸

$$\sum_{(i,j)} \phi_i \cdot (z - \tilde{U}(f, R_\omega))_{i,j} \cdot \phi_j = \sum_{(i,j)} \Phi(R_\omega(\tau^{-1}(i))) \cdot (z - \tilde{U}(f, R_\omega))_{i,j} \cdot \Phi(R_\omega(\tau^{-1}(j))).$$

The evaluation can now also be written using an evaluation functional $\delta_x(f) = f(x)$, so that we have

$$\sum_{(i,j)} \delta_{R_\omega(i)} \left(x \mapsto \delta_{R_\omega(j)} (y \mapsto \Phi(x) \cdot (z - \tilde{U}(f, R_\omega))_{i,j} \cdot \Phi(y)) \right)$$

Secondly we introduce a virtual integration that evaluates the function at the specific positions $R_\omega(i)$. This allows us to conclude equality to the original formulation:

$$(4) = \sum_{(i,j)} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \Phi(x) \cdot (z - \tilde{U}(f, R_\omega))_{i,j} \cdot \Phi(y) \delta_{R_\omega(i)}(dy) \delta_{R_\omega(j)}(dx)$$

Interchanging the order of integration and summation can be done due to linearity. If we now consider the definition of $\tilde{U}(f, R_\omega)_{i,j} = \delta_{ij} \cdot \Sigma(f, i) - f_{i,j}$ from P.2.1 we can write

$$\begin{aligned} \Phi(x) \cdot (z - \delta_{ij} \cdot \Sigma(f, i) + f_{i,j}) \cdot \Phi(y) \\ = \Phi(x) \cdot z \cdot \Phi(y) - \Phi(x) \cdot \delta_{ij} \cdot \Sigma(f, i) \cdot \Phi(y) + \Phi(x) \cdot f_{i,j} \cdot \Phi(y). \end{aligned}$$

With this the integral can be rewritten into a sum of three according to

$$\begin{aligned} z \cdot \int_{\mathbb{R}^d} \Phi(x)^2 \delta_{R_\omega(i)}(dx) - \int_{\mathbb{R}^d} \Phi(x) \cdot \Sigma(f, i) \cdot \delta_{ij} \cdot \Phi(x) \delta_{R_\omega(j)}(dx) \\ + \int_{(\mathbb{R}^d)^2} \Phi(x) \cdot f(x-y) \cdot \Phi(y) (\delta_{R_\omega(i)} \otimes \delta_{R_\omega(j)})(d(x,y)). \end{aligned}$$

Since we still need to perform the summation $\sum_{(i,j) \in [N]^2}$, it comes in handy to include this process in a new definition. For the first integral the \int can be effortlessly interchanged with the third, as it is the case with the last. The second integral still is dependent on the index i , since $\Sigma(f, i) = \sum_{j \in [N] \setminus \{i\}} f_{i,j}$ includes an exclusion of self interaction. It can be rewritten by shifting the summation to $\underline{\Sigma}(f, x) := \sum_{r_* \in \text{im}(R_\omega) \setminus \{x\}} f(x - r_*)$. If x now becomes an element of the image of R_ω , its contribution to the sum is excluded, hence self interaction is still forbidden. With this the integrand becomes independent of the index i and the normalized density measure

⁷This could be done by a summation of particularly defined gaussian functions $x \mapsto a(r_i) \cdot e^{(x-r_i)^2}$, whose amplitudes need to be adjusted recursively for $N \in \mathbb{N}$ points. This will in this thesis not be done explicitly. In the literature this is expressed as *analytically continued* [3, 4].

⁸Again a small warning: Since we make a simplification here, the components $\phi_i \in \mathbb{R}$ need to be drawn from positions $R_\omega(i) \in \mathbb{R}^d$. In a general case one would summarize over $N \cdot d$, but with $\tilde{U}(f, R_\omega)$ having diagonal blocks of $d \times d$ size, a factor of d equal sums can occur. Therefore Φ should originally be a function $\Phi : \mathbb{R} \rightarrow \mathbb{R}$, but with this simplification we decide to use $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ and no further specification of summation domain, whether $[d \cdot N]$ or $[N]$.

$\rho_{R_\omega} := \rho_*^{-1} \cdot \sum_{i \in [N]} \delta_{R_\omega(i)}$ can be introduced.

Definition 2.20. Density Measurement.

Let $R : \Omega \rightarrow V_{d,N}$ be a random variable. Then $\rho_{R_\omega} : \mathcal{B}(\Gamma) \ni A \mapsto \rho_*^{-1} \cdot \sum_{i \in [N]} \delta_{R_\omega(i)}(A)$ is called a *density measure* on $(\Gamma, \mathcal{B}(\Gamma))$ with $\rho_* = N / |V_{d,N}|$.

With this we have generalized the discrete action $\phi \mapsto S_{z,R_\omega}(\phi)$ to a functional action $\Phi \mapsto S_{z,R_\omega}[\Phi]$ and find with virtually unchanged notation

$$S_{z,R_\omega}[\Phi] = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \Phi(x) \cdot (z - \tilde{U}(f, R_\omega)) \cdot \Phi(y) \rho_{R_\omega}(dx) \rho_{R_\omega}(dy) = \text{I} + \text{II} + \text{III},$$

Implicitly it now follows with the introduced summation abbreviation $\underline{\Sigma}(f, x) = \sum_{r_* \in \text{im}(R_\omega) \setminus \{x\}} f(x - r_*)$ that

$$\text{I} = \rho_* \cdot z \cdot \int_{V_{d,N}} \Phi(x)^2 \rho_{R_\omega}(dx) \quad (5)$$

$$\text{II} = -\rho_* \cdot \int_{V_{d,N}} \Phi(x) \cdot \underline{\Sigma}(f, x) \cdot \Phi(x) \rho_{R_\omega}(dx) \quad (6)$$

$$\text{III} = \rho_*^2 \cdot \int_{(V_{d,N})^2} \Phi(x_1) \cdot f(x - y) \cdot \Phi(x_2) (\rho_{R_\omega} \otimes \rho_{R_\omega})(dx). \quad (7)$$

Note that from the form of the Gaussian density $\Phi \mapsto \mathcal{G}_{R_z(\tilde{U}(f, R_\omega))}[\Phi]$ (see equation (3)) we need to carry along a factor of $-1/2$ in front of the action functional. Looking now at the form of the Green's function G_N we can see the appearance of the action functional S_{z,R_ω} and the density measure ρ_{R_ω} :

$$\int_{V_{d,N}} \left[\int_{(\mathbb{R}^d)^2} e^{i \cdot \langle p, x - y \rangle} \cdot \overbrace{\left(\int_{\mathcal{F}_{d,N}} \frac{\Phi(x) \cdot \Phi(y)}{I_{\tilde{U}(f, r_*)}(z)} \underbrace{\mathcal{G}_{\tilde{U}, z, r_*}(d\Phi)}_{\text{includes } S_{z,r_*}} \right)}^{\text{extrapolated}} \underbrace{(\rho_{r_*} \otimes \rho_{r_*})(d(x, y))}_{\text{density}} \right] \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*),$$

where within the gaussian *functional* measure $\mathcal{G}_{\tilde{U}, z, r_*}$ our action S_{z,r_*} is hidden.

Also notice, that we silently interchanged the well known integration on $\text{TF}(V_{d,N}, r_*)$ or in the large volume limit simply \mathbb{R}^d with a *functional integral* of $\Phi \mapsto \Phi(x) \cdot \Phi(y) \cdot \exp(-1/2 \cdot S_{z,r_*}(\Phi))$ with a much less defined domain $\mathcal{F}_{d,N}$ and measure \mathcal{D} . To the physicists this is well handled, since we “in the end only need to know values at $\Phi(r_*(i))$ ”, which themselves were well defined by ϕ_i . But since it is everything else but simple to imagine a measure of functions in a not well defined domain, discussion is needed. But at this point we will not go into further detail, since the main goal is to *use* the derived action functional.

We now want to organize the integrals of S_{z,r_*} in a way that we have a free theory and a interaction theory at hand. This can be done by shifting the used measure ρ_{r_*} to a free and a fluctuating part.

Definition 2.21. Change of Measures.

Let for $R : \Omega \rightarrow V_{d,N}$ the measure $\rho_{R(\omega)}$ be defined by 2.20, then $\delta\rho_{R(\omega)} : \mathcal{B}(\Gamma) \rightarrow \mathbb{R}$ introduces a measure for density disorder in the system by the definition $\rho_{R(\omega)} = \square_{R(\omega)} + \delta\rho_{R(\omega)}$ for a measure $\square_{R(\omega)} : \mathcal{B}(\Gamma) \rightarrow \mathbb{R}_{\geq 0}$.^a

^aSince we do not need many characteristics of the ordered measure $\square_{R(\omega)}$, we choose for it an arbitrary symbol. (By its symmetry it sort of represents what we want it to represent.)

Utilizing this change in measures we can sort the previously defined action functional summands according to the appearance of density fluctuations measures. For this we aim to formulate terms \bar{I} , \bar{II} and \bar{III} by applying the change and rearranging terms once more. For the first summand I this results in

$$I = -\frac{\rho_*}{2} \cdot \left(\int_{(V_{d,N})^2} z \cdot \Phi(x)^2 (\square_{R_\omega})(dx) + \int_{(V_{d,N})} \Phi(x)^2 \delta\rho_{R_\omega}(dx) \right),$$

and analogously for II and III, whilst putting $F(x) := \rho_* \cdot \Phi(x_1) \cdot f(x_1 - x_2) \cdot \Phi(x_2)$ for readability:

$$\begin{aligned} II &= \frac{\rho_*}{2} \cdot \left(\int_{(V_{d,N})} \Phi(x)^2 \cdot \underline{\Sigma}(f, x) (\square_{R_\omega})(dx) + \int_{(V_{d,N})} \Phi(x)^2 \cdot \underline{\Sigma}(f, x) \delta\rho_{R_\omega}(dx) \right), \\ III &= -\frac{\rho_*^2}{2} \cdot \left(\int_{(V_{d,N})^2} F(x) ((\square_{R_\omega}) \otimes (\square_{R_\omega}))(dx) \right. \\ &\quad \left. + 2 \cdot \int_{(V_{d,N})^2} F(x) ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})(dx) \right. \\ &\quad \left. + \int_{(V_{d,N})^2} F(x) ((\delta\rho_{R_\omega} \otimes \delta\rho_{R_\omega}))(dx) \right). \end{aligned}$$

Now a simple sort of terms regarding the appearance of a density fluctuation (measure) yields three integral terms, which represent the *interaction-free* part without any density fluctuations and the *interactive* part with either one or two density fluctuations. Its physical nature can be found in scattering events, where disorders in the medium result in density fluctuations.

During sorting the definition of *vertices* $V_{f,\bar{I}}$, $V_{f,\bar{II}}$ and $V_{f,\bar{III}}$ comes handy, which later on in their fourier representation will dictate the form of the feynman diagrams. Their explicit definition can be read from matching integrands to integrals with equal density measures after sorting. Following this we can note the definitions for the action functional summands:

$$\bar{I} := \int_{(V_{d,N})^2} \Phi(x) \cdot V_{f,\bar{I}}(x, z) \cdot \Phi(y) (\square_{R_\omega})^2(d(x, y)), \quad (8)$$

$$\bar{II} := \int_{(V_{d,N})^2} \Phi(x) \cdot V_{f,\bar{II}}(x) \cdot \Phi(y) ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})(d(x, y)), \quad (9)$$

$$\bar{III} := \int_{(V_{d,N})^2} \Phi(x) \cdot V_{f,\bar{III}}(x) \cdot \Phi(y) (\delta\rho_{R_\omega})^2(d(x, y)). \quad (10)$$

Concluding this derivation we have found the action functional summands \bar{I} , \bar{II} and \bar{III} as the *interaction-free* and *interactive* parts of the action functional, which will be used to define the

moment generating function Z_{z,R_ω} .

Corollary 2.2. The Functional of Action.

The action functional S_{z,R_ω} is constituted by the *free action* summand $S_{z,R_\omega}^{(0)}$ given by the term \bar{I} and an *interacting action* summand $S_{z,R_\omega}^{(int)}$ given by the term $\bar{\Pi} + \bar{\Pi\!I\!I}$ as $S_{z,R_\omega} = S_{z,R_\omega}^{(0)} + S_{z,R_\omega}^{(int)}$.

On the other hand this field shift also impacts the definition of G_N in equation (3), as there appear two measures ρ_{R_ω} that need to be adjusted. Doing so yields three components of G_N of the following forms, where $\iiint := \int_{V_{d,N}} \int_{(\mathbb{R}^d)^2} \int_{\mathcal{F}_{d,N}}$ is used:

$$\begin{aligned} G_N^{(0)}(p, z) &= \iiint \exp(\hat{i} \cdot \langle p, x - y \rangle) \cdot \frac{\Phi(x) \cdot \Phi(y)}{I_{\tilde{U}(f,r_*)}} \mathbb{G}_{\tilde{U},z,r_*}(d\Phi) (\square_{R_\omega})^2(d(x,y)) \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*), \\ G_N^{(1)}(p, z) &= 2 \cdot \iiint \exp(\hat{i} \cdot \langle p, x - y \rangle) \cdot \frac{\Phi(x) \cdot \Phi(y)}{I_{\tilde{U}(f,r_*)}} \mathbb{G}_{\tilde{U},z,r_*}(d\Phi) ((\square_{R_\omega}) \otimes \delta\rho_{r_*})(d(x,y)) \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*), \\ G_N^{(2)}(p, z) &= \iiint \underbrace{\exp(\hat{i} \cdot \langle p, x - y \rangle) \cdot \frac{\Phi(x) \cdot \Phi(y)}{I_{\tilde{U}(f,r_*)}}}_{\text{resolvent Fouriercoefficients}} \underbrace{\mathbb{G}_{\tilde{U},z,r_*}(d\Phi) (\delta\rho_{r_*})^2(d(x,y)) \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*)}_{\text{measures}}. \end{aligned}$$

Also the definitions $\mu_{\bar{I}} := (\square_{R_\omega})^2$, $\mu_{\bar{\Pi}} := ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})$ and $\mu_{\bar{\Pi\!I\!I}} := (\delta\rho_{R_\omega})^2$ can now be introduced for the three density fluctuation measures. This will enhance readability later on. If we now write down the expected value according to the literature notation [4, 3], we get for the first term

$$G_N^{(0)}(p, z) = \int_{V_{d,N}} \int_{(\mathbb{R}^d)^2} \frac{\exp(\hat{i} \cdot \langle p, x - y \rangle)}{I_{\tilde{U}(f,r_*)}} \cdot \langle \Phi(x) \cdot \Phi(y) \rangle_{\mathbb{G}_{\tilde{U},z,r_*}} (\square_{R_\omega})^2(d(x,y)) \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*).$$

The interesting part that needs to be remembered at all times during the development is the existence of *two* independent measures. For the third term this will get obvious, as the density fluctuation measure $\delta\rho_{r_*}$ appears twice:

$$\int_{V_{d,N}} \int_{(\mathbb{R}^d)^2} eI(r_*, p, x, y) \cdot \overbrace{\langle \Phi(x) \cdot \Phi(y) \rangle_{\mathbb{G}_{\tilde{U},z,r_*}}}^{(i)} \underbrace{(\delta\rho_{r_*} \otimes \delta\rho_{r_*})(d(x,y)) \left(\frac{\lambda_R}{|V_{d,N}|} \right) (dr_*)}_{(ii)}.$$

As one can see we have to evaluate the expected value regarding $\mathbb{G}_{\tilde{U},z,r_*}$ and the product $\Phi(x) \cdot \Phi(y)$ in (i) and another expected value regarding $\delta\rho_{r_*} \otimes \delta\rho_{r_*}$ with respect to $\lambda_R / |V_{d,N}|$ in (ii). This is the result of the systems hamiltonian, which itself is a function $(r_*, \phi) \mapsto \mathcal{H}(r_*, \phi)$ that was defined to be part of the density $\exp(-\beta \cdot \mathcal{H}(r_*, \phi))$ of \mathbb{P} in our probability space $(\Omega, \Sigma, \mathbb{P})$. This splitting of measures $\mathbb{P}(r_*, \phi) = P_r + P_\phi$ a motive all along the derivation, starting with the initial definition of the hamiltonian and the description using equillibrium positions and independent fluctuations. So, even though we manipulated and expanded the original integral $\int_{\Omega} 1 \mathbb{P}$ from the introduction and introduced the resolvent formalism, still the underlying physical system remains the same but formed in a more delightful way for perturbation theory.

We now want to take a closer look at the exponential of our action functional and how it can be manipulated to start a perturbative expansion.

2.3.1 Operator Generated MGF

As we can already see at this point the gaussian exponential of the action functional S_{z,R_ω} can be disassembled into $\exp(-S_{z,R_\omega}/2) = \exp(-S_{z,R_\omega}^{(0)}/2) \cdot \exp(-S_{z,R_\omega}^{(int)}/2)$ so that we can write

$$\int_{\mathcal{F}_{d,N}} \exp(-S_{z,R_\omega}[\Phi]/2) \mathcal{D}(d\Phi) = \int_{\mathcal{F}_{d,N}} \exp\left(-S_{z,R_\omega}^{(0)}[\Phi]/2\right) \cdot \exp\left(-S_{z,R_\omega}^{(int)}[\Phi]/2\right) \mathcal{D}(d\Phi).$$

A cleverly designed way of introducing a *field shift* will allow us to formulate the interactive part of this integrand using the non-interactive part. For this we need to specify a crafted operator $\text{Ex}(\ell_f)$ that fulfills the relation

$$\mathcal{F}_{d,N} \ni \Phi \mapsto \exp(S_{z,R_\omega}^{(int)}[\Phi]) = \text{Ex}(\ell_f) \circ (S_{z,R_\omega}^{(0)} \Phi).$$

In this again the notation changed minorly, since now $S_{z,R_\omega}^{(0)} \Phi : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathbb{C}$ is an external field extension of the action functional $S_{z,R_\omega}^{(0)}$. This becomes clearer by the following definition.

Definition 2.22. External Field Shifting.

Let $R \in (\Omega \rightarrow V_{d,N})$ and $\Phi \in \mathcal{F}_{d,N}$ be the system parameters. For $z \in \mathbb{C}$ and $J \in \mathcal{S}(\mathbb{R}^d)$ we define

$$S_{z,R_\omega}^{(0)} \Phi : J \mapsto -\frac{1}{2} \cdot S_{z,R_\omega}^{(0)}[\Phi] + \frac{\overset{\circ}{i}}{2} \cdot \int_{\mathbb{R}^d} J(x) \cdot \Phi(-x) + J(-x) \cdot \Phi(x) \lambda(dx)$$

as the *external field shift* to the free theory action $S_{z,r_\omega}^{(0)}[\Phi]$.

A neat characteristic of this shifting is that we can recover the initial gaussian exponent as $(S_{z,R_\omega} \Phi)^{(0)}(0) = -S_{z,R_\omega}^{(0)}[\Phi]/2$, which will soon be of great use. Since we can further write $S_{z,R_\omega}^{(int)}[\Phi] = \bar{\Pi} + \bar{\Pi}\bar{\Pi}$ we can handle the summands individually. For the first summand, namely $\bar{\Pi}$, let $I_z : \Gamma^2 \rightarrow \mathbb{R}$ be defined such that $\bar{\Pi} = \int_{\Gamma^2} I_z \mu_{\bar{\Pi}}$ holds. We now intend to represent I_z in a form that uses a functional theoretical approach formally discussed in literature⁹ and briefly in the Appendix. Right now we only need

$$\frac{\delta}{\delta J(\xi)} (S_{z,r_\omega}^{(0)} \Phi)[J] = \int_{\mathbb{R}^d} \frac{\overset{\circ}{i}}{2} \cdot \Phi(-x) \cdot \frac{\delta}{\delta J(\xi)} J(x) \lambda(dx) + \int_{\mathbb{R}^d} \frac{\overset{\circ}{i}}{2} \cdot \Phi(x) \cdot \frac{\delta}{\delta J(\xi)} J(-x) \lambda(dx).$$

Following T.?? we can use $\frac{\delta}{\delta J(\xi)} J(x) = \delta(x - \xi)$ to obtain

$$\frac{\delta}{\delta J(\xi)} (S_{z,r_\omega}^{(0)} \Phi)[J] = \frac{\overset{\circ}{i}}{2} \cdot \Phi(-\xi) + \frac{\overset{\circ}{i}}{2} \cdot \Phi(-\xi) = \overset{\circ}{i} \cdot \Phi(-\xi). \quad (11)$$

⁹See for example [12]. Other possible sources are several scripts from courses on functional analysis or mathematical physics, which are not explicitly mentioned in this thesis.

Now the application of this formula to the integrand I_z yields

$$\begin{aligned} I_z(x) &= \Phi(x_1) \cdot V_{f,\bar{\Pi}}(x, z) \cdot \Phi(x_2) \\ &= \left(\underbrace{\left[(-1) \cdot \frac{\delta}{\delta J(-x_1)}(\cdot) \cdot V_{f,\bar{\Pi}}(x) \cdot \frac{\delta}{\delta J(-x_2)}(\cdot) \right]}_{=: \mathcal{O}_{f,\bar{\Pi}}(x)} S_{z,R_\omega} \Phi \right) [J], \end{aligned}$$

in which we have introduced the operator $\mathcal{O}_{f,\bar{\Pi}}(x)$ acting on the functional $J \mapsto (S_{z,R_\omega} \Phi)[J]$ with the external field J . This allows us to rewrite the first term of interaction only using the free theory result:

$$\bar{\Pi} = \underbrace{\left[\int_{\Gamma^2} \mathcal{O}_{f,\bar{\Pi}}(x) \mu_{\bar{\Pi}}(dx) \right]}_{=: \ell_{f,\bar{\Pi}}} S_{z,R_\omega} \Phi[J].$$

As one can already imagine, the same procedure for $\bar{\Pi}\bar{\Pi}$ leads to a similar form of $\ell_{f,\bar{\Pi}\bar{\Pi}}$, where only $V_{f,\bar{\Pi}\bar{\Pi}}$ appears instead of $V_{f,\bar{\Pi}}$. Combination yields

$$\bar{\Pi} + \bar{\Pi}\bar{\Pi} = \underbrace{\left[\ell_{f,\bar{\Pi}} + \ell_{f,\bar{\Pi}\bar{\Pi}} \right]}_{=: \ell_f} (S_{z,R_\omega} \Phi)[J].$$

This now already looks promising for our operator $\text{Ex}(\ell_f)$. Looping back to the beginning we obtain for the interactive exponential

$$\int_{\mathcal{F}_{d,N}} \exp(S_{z,R_\omega}[\Phi]) \mathcal{D}(d\Phi) = \int_{\mathcal{F}_{d,N}} \exp((S_{z,R_\omega}^{(0)} \Phi)[J]) \cdot \exp((\ell_f S_{z,R_\omega} \Phi)[J]) \mathcal{D}(d\Phi) \Big|_{J=0}.$$

In a last step we need to change a small detail in the first definition of $\mathcal{O}_{f,\bar{\Pi}}$. Because we have an exponential function, the derivative $\frac{\delta}{\delta J(-x_1)}$ by chain rule will result in the same factor $\exp((S_{z,R_\omega}^{(0)} \Phi)[J])$ that we provided initially, such that the second derivative $\frac{\delta^2}{\delta J(-x_2)}$ can be applied to the first derivatives result. In contrast, it was *multiplied* with the exponential function in the first definition and would result in a wrong factor. Since multiplication of Functionals can also be interpreted as composition of operators, this might seem not to be a big deal, but its implications to the definition of Ex are crucial. It implies a parallel definition of $\mathcal{L}_f := \mathcal{L}_{f,\bar{\Pi}} + \mathcal{L}_{f,\bar{\Pi}\bar{\Pi}}$ with $\mathcal{L}_{f,\bar{\Pi}} := \int_{\Gamma^2} \mathcal{O}_{f,\bar{\Pi}}^\circ(x) \mu_{\bar{\Pi}}(dx)$ and $\mathcal{O}_{f,\bar{\Pi}}^\circ(x) := -V_{f,\bar{\Pi}}(x) \cdot \frac{\delta}{\delta J(-x_1)} \circ \frac{\delta}{\delta J(-x_2)}$ (for $\mathcal{L}_{f,\bar{\Pi}\bar{\Pi}}$ analogously). With these definitions each derivative application yields a Φ and the corresponding vertex function, as well as preserving the exponential factor. This allows us to write

$$\sum_{n=0}^{\infty} \frac{1}{n!} \cdot ((\ell_f S_{z,R_\omega} \Phi)[J])^n \cdot \exp((S_{z,R_\omega}^{(0)} \Phi)[J]) = \sum_{n=0}^{\infty} \frac{1}{n!} \cdot \mathcal{L}_f^n (\exp((S_{z,R_\omega}^{(0)} \Phi)))[J]$$

where $\text{Ex}(\mathcal{L}_f)$ finally is defined by the right hand side and the application to $J \mapsto \exp((S_{z,R_\omega}^{(0)} \Phi)[J])$.¹⁰

¹⁰We do not discuss convergence of this series, since it would require again a much more detailed discussion of the occurring objects in question.

Postulate 2.4. The Moment Generating Function.

Let $J \mapsto (S_{z,R_\omega}^{(0)} \Phi)[J]$ be an external field shift on $\mathcal{S}(\mathbb{R}^d)$ according to 2.22 and $\mathbb{G}_{\tilde{U}, z, R_\omega, J} := (\Phi \mapsto (S_{z,R_\omega}^{(0)} \Phi)[J]) \cdot \mathcal{D}$ the field extended gaussian functional measure. Let \mathcal{L}_f be the Lagrange operator defined as shown above, then there exists a functional $\text{Ex}(\mathcal{L}_f)$ such that^a (neglecting measures)

$$\underbrace{\text{Ex}_{\mathcal{L}_f} \left[J \mapsto \int_{\mathcal{F}_{d,N}} e^{(S_{z,R_\omega}^{(0)} \Phi)[J]} d\Phi \right] [J]}_{=: Z_{z,R_\omega}^{(0)}} = \int_{\mathcal{F}_{d,N}} e^{(S_{z,R_\omega} \Phi)[J]} d\Phi =: Z_{z,R_\omega}[J].$$

We call the resulting $J \mapsto Z_{z,R_\omega}[J]$ the *moment generating function* of the corrected ERM model.

^aWe have implicitly stated $(S_{z,R_\omega} \Phi)[J] = (S_{z,R_\omega}^{(0)} \Phi)[J] + S_{z,R_\omega}^{(int)}[\Phi]$.

This procedure can also be done in the Fourier domain, which is object to the next chapters investigation.

2.3.2 Representation of the Action using its Fourier Transform

Looking at the free theory summand of the action functional defined in equation (8) the bare propagator can already be defined, which in the high density limit $\rho_* \rightarrow \infty$ already fully describes the resolvent G_N . As we will see below, it already has the form of our resolvent result from the *Dyson* fixed point equation in definition 2.28 for vanishing self energy $\Sigma = 0$ [3]. This is going to be discussed again after developing the Dyson formalism later on. But first we are going to derive its form by writing

$$\bar{I} = \int_{(V_{d,N})^2} (\mathcal{F}^{-1}(\mathcal{F}\Phi))(x_1) \cdot V_{f,\bar{I}}(x, z) \cdot (\mathcal{F}^{-1}(\mathcal{F}\Phi))(x_2) \lambda(dx).$$

Using the definition of \mathcal{F}^{-1} from 2.12 and writing $\hat{\Phi} := \mathcal{F}\Phi$ it follows

$$\bar{I} = \int_{(V_{d,N})^2} \int_{(\mathbb{R}^d)^2} \hat{\Phi}(p_1) \cdot e^{-\hat{i} \cdot \langle p_1, x_1 \rangle} \cdot V_{f,\bar{I}}(x, z) \cdot \hat{\Phi}(p_2) \cdot e^{-\hat{i} \cdot \langle p_2, x_2 \rangle} \lambda(dx) \lambda(dp).$$

Looking at the Vertex function $V_{f,\bar{I}}(x, z) = ((z - \rho_* \cdot \hat{f}(0) \cdot \mathbb{1}_{\{x_1\}})(x_2) + \rho_* \cdot f(x_1 - x_2))$ we can rearrange the integral while neglecting $\Phi(p_1) \cdot \Phi(p_2)$ for a second to get

$$\int_{\mathbb{R}^d} e^{-\hat{i} \cdot \langle x_2, p_2 \rangle} \cdot \underbrace{\left[\int_{\mathbb{R}^d} e^{-\hat{i} \cdot \langle x_1, p_1 \rangle} \cdot (z - \rho_* \cdot \hat{f}(0)) \delta_{x_2}(dx_1) + \int_{\mathbb{R}^d} e^{-\hat{i} \cdot \langle x_1, p_1 \rangle} \cdot \rho_* \cdot f(x_1 - x_2) \lambda(dx_1) \right]}_{(z - \rho_* \cdot \hat{f}(0)) \cdot \exp(-\hat{i} \cdot \langle x_2, p_1 \rangle)} \lambda(dp).$$

The second summand can be solved by multiplication with $\exp(-\hat{i} \cdot \langle x_2 - x_1, p_1 \rangle)$ to get

$$e^{-\hat{i} \cdot \langle x_2, p_1 \rangle} \cdot \rho_* \cdot \int_{\mathbb{R}^d} f(x_1 - x_2) \cdot e^{-\hat{i} \cdot \langle x_1 - x_2, p_1 \rangle} \lambda(dx_1) = e^{-\hat{i} \cdot \langle x_2, p_1 \rangle} \cdot \rho_* \cdot \hat{f}(p_1).$$

In the big picture we now can write the first term \bar{I} as

$$\bar{I} = \int_{\mathbb{R}^d} \hat{\Phi}(p_1) \cdot \hat{\Phi}(p_1) \cdot (z - \rho_* \cdot \hat{f}(0) + \rho_* \cdot \hat{f}(p_1)) \cdot \int_{V_{d,N}} \exp(-i \cdot \langle x_2, p_1 + p_2 \rangle) \lambda(dx_2) \lambda(dp).$$

Because of the divergence of the integral $p_1 + p_2 \mapsto \int_{V_{d,N}} \exp(-i \cdot \langle x_2, p_1 + p_2 \rangle) \lambda(dx_2)$ for all $p_1 + p_2 \neq 0$ we can conclude the conservation of momentum in the system, which directly means $p_1 = -p_2$. Therefore we find

$$\bar{I} = \int_{\mathbb{R}^d} \hat{\Phi}(p) \cdot (z - \rho_* \cdot (\hat{f}(0) - \hat{f}(p))) \cdot \hat{\Phi}(-p) \lambda(dp),$$

in which the inverse bare propagator $G_0(p, z)$ can be found!

Definition 2.23. The Propagator.

Let $f \in \mathcal{S}(\mathbb{R}^d)$ and $\rho_* \in \mathbb{R}$, then we define the *free or bare propagator* $G_0 : \mathbb{R}^d \times \mathbb{C} \rightarrow \mathbb{R}$ by

$$G : (p, z) \mapsto \frac{1}{z - \rho_* \cdot (\hat{f}(0) - \hat{f}(p))}.$$

The mapping $p \mapsto \rho_* \cdot (\hat{f}(0) - \hat{f}(p))$ further describes the *bare dispersion relation*.

Within the theory of high density this already represents the resolvent introduced in Postulate 2.2. The same procedure on \bar{II} and \bar{III} following [3, 4] gives rise to the *vertex functions* V and μ_z . We will not discuss the details of this derivation, since it follows the same idea and can be seen in literature [3]. The important corollaries from it are the definition of the two vertex functions in the Fourier domain.

Theorem and Definition 2.2. The Vertex Function.

The vertex function is given by $V(q, p) := \rho_* \cdot (\hat{f}(q) - \hat{f}(q - p))$. It has the symmetries $V(q, p) = V(-q, -p)$ and $V(q, p) = -V(p - q, p)$.

Proof. Let $p, q \in \mathbb{R}^d$. Then from definition and the rotational symmetry $\hat{f}(-q) = \hat{f}(q)$ stated in D.2.17 we get

$$V(-q, -p) = \rho_* \cdot (\hat{f}(-q) - \hat{f}(-q + p)) = \rho_* \cdot (\hat{f}(q) - \hat{f}(q - p)) = V(q, p).$$

For the second symmetry we calculate

$$-V(p - q, p) = -\rho_* \cdot (\hat{f}(p - q) - \hat{f}(p)) = \rho_* \cdot (\hat{f}(q) - \hat{f}(q - p)) = V(q, p).$$

This concludes the proof. q.e.d.

The arguments of the vertex function describe the transfer of moments during a scattering

event. It is visually much more clear in the diagrammatical representation given later on in the Feynman rules, see D.2.27.

Theorem and Definition 2.3. Three Point Fourier Vertex.

Given by $\mu(p, q) := G_0(p, z)^{-1} + V(q, p)$, where V is the vertex function from 2.2. It has the symmetry $\mu(p, q) = \mu(-p, -q)$.

Proof. The stated symmetries follow directly from theorem 2.2 and $G_0(-p, z) = G_0(p, z)$.

q.e.d.

Again we can assign physical meaning to the vertex' arguments: The first momentum describes the incoming mode, the second to the corresponding density fluctuation [4]. This can be again visually seen later on in the Feynman diagram's three point node defined in 2.26. With those definitions we are able to express the summands of the Fourier action as in the following corollary 2.3.

Corollary 2.3. Propagator-notation of \mathbb{S} .

Let \mathbb{S} be a functional of $\Phi_{\varphi, r_\omega, f}$ and G_0 the free propagator. Then we can write $\mathbb{S} = \bar{\mathbf{I}} + \bar{\mathbf{II}} + \bar{\mathbf{III}}$ with

$$\begin{aligned}\bar{\mathbf{I}} &= \int_{\mathbb{R}^d} \hat{\Phi}_\varphi(p) \cdot G_0(p, z)^{-1} \cdot \hat{\Phi}_\varphi(-p) \, \lambda(dp), \\ \bar{\mathbf{II}} &= \int_{(\mathbb{R}^d)^2} \hat{\Phi}_\varphi(p_1) \cdot \mu(p_1, p_2) \cdot \hat{\Phi}_\varphi(-p_1 - p_2) \left(\lambda \otimes (2\pi)^{-1} \cdot \delta\rho_{r_\omega} \right)(dp), \\ \bar{\mathbf{III}} &= \int_{R(d,3)} \hat{\Phi}_\varphi(p_1) \cdot V(p_3, -p_2) \cdot \hat{\Phi}(p_3) \left((2\pi)^{-1} \cdot \delta\rho_{r_\omega} \right)^2(dp),\end{aligned}$$

where $R(d, 3) := \{x \in (\mathbb{R}^d)^3 : x_1 + x_2 + x_3 = 0\}$ is the restricted hyperplane^a in $(\mathbb{R}^d)^3$. Furthermore we define $\mu(p_1, p_2) := G_0(p_1, z)^{-1} \cdot V(p_2, -p_1)$ and $V(p_3, -p_2) := \rho \cdot (\hat{f}(p_3) - \hat{f}(p_3 + p_2))$.

^aOne can also imagine occurring δ within integration as *restrictions* towards the integration domain.

2.4 Approximation of the Moment Generating Function

With postulate (2.4) we have layed the groundwork for the practical calculation method. For it to unleash we write the operator (\mathcal{L}_f) in its series expansion by assumption of convergence to

$$Z_{z, R_\omega}[J] = \text{Ex}_{\mathcal{L}_f} \left[Z_{z, R_\omega}^{(0)} \right] [J] = \sum_{n \in \mathbb{N}} \frac{1}{n!} \cdot \mathcal{L}_f^n(Z_{z, R_\omega}^{(0)})[J].$$

Stepping back and looking at the *propagator-notation* of $\bar{\mathbf{I}}$ following our results in 2.3 we can evaluate the free action under field shifting given by $S_{z, r_\omega}^{(0)} \Phi$ using its *propagator representation*

as

$$(S_{z,r_\omega}^{(0)} \Phi_\varphi)[J] = \int_{\Gamma^2} -\hat{\Phi}_\omega(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\omega(-p) + \hat{J}(p) \cdot \hat{\Phi}_\omega(-p) + \hat{J}(-p) \cdot \hat{\Phi}_\omega(p) \lambda(dp).$$

Within this object we now work with the fourier transformed field of forces according to our Definition of Fourier transform in 2.12. Recalling the definition of $Z_{r,r_\omega}^{(0)}$, we can perform a formal linear translation of integration variables according to $\mathcal{T}(\hat{\Phi}_\varphi) := \hat{\Phi}_\varphi + \hat{J} \cdot G_0(\cdot, z)$ for $\mathcal{T} : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d)$ and given $z \in \mathbb{C}$. This approach yields in first application

$$\begin{aligned} & -(\hat{\Phi}_\varphi + \hat{J} \cdot G_0(\cdot, z))(p) \cdot G_0(p,z)^{-1} \cdot (\hat{\Phi}_\varphi + \hat{J} \cdot G_0(\cdot, z))(-p) \\ & + \hat{J}(p) \cdot (\hat{\Phi}_\varphi + \hat{J} \cdot G_0(\cdot, z))(-p) + \hat{J}(-p) \cdot (\hat{\Phi}_\varphi + \hat{J} \cdot G_0(\cdot, z))(p). \end{aligned}$$

One can now expand this expression by distributive multiplication to reveal

$$\begin{aligned} & = -\hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) - \hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{J}(-p) \cdot G_0(-p,z) \\ & - \hat{J}(p) \cdot G_0(p,z) \cdot G_0(-p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) \\ & - \hat{J}(p) \cdot G_0(p,z) \cdot G_0(-p,z)^{-1} \cdot \hat{J}(-p) \cdot G_0(-p,z) \\ & + \hat{J}(p) \cdot \hat{\Phi}_\varphi(-p) + \hat{J}(p) \cdot \hat{J}(-p) \cdot G_0(-p,z) \\ & + \hat{J}(-p) \cdot \hat{\Phi}_\varphi(p) + \hat{J}(-p) \cdot \hat{J}(p) \cdot G_0(p,z) \\ & = -\hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) - \hat{J}(-p) \cdot [G_0(p,z)^{-1} \cdot G_0(-p,z)] \cdot \hat{\Phi}_\varphi(p) \\ & - \hat{J}(p) \cdot 1 \cdot \hat{\Phi}_\varphi(-p) - \hat{J}(p) \cdot G_0(-p,z) \cdot \hat{J}(-p) \\ & + \hat{J}(p) \cdot \hat{\Phi}_\varphi(-p) + \hat{J}(p) \cdot G_0(-p,z) \cdot \hat{J}(-p) \\ & + \hat{J}(-p) \cdot \hat{\Phi}_\varphi(p) + \hat{J}(-p) \cdot G_0(p,z) \cdot \hat{J}(p). \end{aligned}$$

We can immediately see $\hat{J}(\pm p) \cdot \hat{\Phi}_\varphi(\mp p)$ cancelling out with its counterparts as well as $\hat{J}(p) \cdot G_0(-p,z) \cdot \hat{J}(-p)$. To finalize the cancelling we have to prove $G_0(p,z)^{-1} \cdot G_0(-p,z) = 1$, which follows from discussing the Fourier transform of f given as a *radial symmetric* function, i.e. $f(p) = f_{||}(\|p\|_2)$ for $p \in \mathbb{R}^d$, such that $\hat{f}(p) = \int_{\mathbb{R}^d} f_{||}(\|-x\|_2) \cdot \exp(i \cdot \langle p, -x \rangle) \lambda(dx) = \hat{f}(-p)$ preserves symmetry. Remembering $G_0(p,z) = z - \rho_* \cdot (\hat{f}(0) - \hat{f}(p))$ we can directly see the result. Therefore we can establish the integrand of $(S_{z,r_\omega}^{(0)} \Phi_\varphi)[J]$ as

$$-\hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) + \hat{J}(p) \cdot G_0(p,z) \cdot \hat{J}(-p).$$

Integrating this expression with respect to $p \in \mathbb{R}^d$ we can split up via linearity to reveal

$$\begin{aligned} & \int \exp\left(-\frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) \lambda(dp)\right. \\ & \quad \left. + \frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{J}(p) \cdot G_0(p,z) \cdot \hat{J}(-p) \lambda(dp)\right) \mathcal{D}(d\Phi_\varphi). \end{aligned}$$

Because of the invariance of the second summand in the exponential we interchange its position

with the functional integral to achieve a scaled gaussian integral of the form

$$Z_{z,r_\omega}^{(0)}[J] = \exp\left(\frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{J}(p) \cdot G_0(p,z) \cdot \hat{J}(-p) \lambda(dp)\right) \cdot \int \exp\left(-\frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) \lambda(dp)\right) \mathcal{D}(d\Phi_\varphi).$$

This means that $Z_{r,r_\omega}^{(0)}[0] = 1$ is given by the normalization factor coming from the gaussian integral

$$N_{Z_0,z} := \int e^{-\frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{\Phi}_\varphi(p) \cdot G_0(p,z)^{-1} \cdot \hat{\Phi}_\varphi(-p) \lambda(dp)} \mathcal{D}(d\Phi_\varphi) \in \mathbb{R}$$

such that $Z_{r,r_\omega}^{(0)}[J]$ becomes proportional to the standalone exp component[11]. Therefore we have our first result for the *basis* of our perturbative expansion of the moment generating function.

Corollary 2.4. Perturbative Basis of the MGF with Normalization.

Let $\text{Ex}(\mathcal{L}_f)$ be the development operator for the generating function $Z_{z,R_\omega}[J]$. Then its free theory argument $Z_{z,R_\omega}^{(0)}[J]$ can be written as

$$Z_{z,R_\omega}^{(0)}[J] = \exp\left(-\frac{1}{2} \cdot \int_{\mathbb{R}^d} \hat{J}(p) \cdot G_0(p,z) \cdot \hat{J}(-p) \lambda(dp)\right) \cdot N_z^{(0)}.$$

Assuming $N_z^{(0)} \in \mathbb{R}_{\neq 0}$ the *normalization factor* enforces the initial value $Z_{z,R_\omega}^{(0)}[0] = 1$.

With the free theory under Fourier transformation explicitly handled, the two interactive summands now include the two newly introduced vertices V and μ_z . The construction of Ex however remains similar in the Fourier image. With this and [4] we therefore find:¹¹

$$\begin{aligned} \mathcal{L}_{f,\overline{\Pi},\mathcal{F}} &:= \int_{(\mathbb{R}^d)^2} \mu_z(p) \cdot \left(\frac{\delta}{\delta J(-p_1)} \circ \frac{\delta}{\delta J(-p_1 - p_2)} \right)(\cdot) \bar{\mu}_{\overline{\Pi}}(dp), \\ \mathcal{L}_{f,\overline{\Pi\Pi},\mathcal{F}} &:= \iiint_{\delta\rho_{134}(\mathbb{R}^d)} V_z(p_3, -p_2) \cdot \left(\frac{\delta}{\delta J(-p_1)} \circ \frac{\delta}{\delta J(-p_3)} \right)(\cdot) \bar{\mu}_{\overline{\Pi\Pi}}(dp). \end{aligned}$$

Notice how we can now connect the generating function to our main object of interest, the resolvent. Since expressed with extrapolated gaussian density, the resolvent involves a factor $\Phi(x) \cdot \Phi(y)$ combined with the density $\Phi \mapsto \exp(S_{z,R_\omega}[\Phi])$, we can extend the integral using the same field shifting technique to

$$\begin{aligned} &\int_{\mathcal{F}_{d,N}} \Phi(x) \cdot \Phi(y) \cdot \exp((S_{z,R_\omega}\Phi)[J]) \lambda(d\Phi) \\ &\quad = \int_{\mathcal{F}_{d,N}} \left(\frac{\delta}{\delta J(-x)} \circ \frac{\delta}{\delta J(-y)} \right) \cdot \exp((S_{z,R_\omega}\Phi)[J]) \lambda(d\Phi). \end{aligned} \quad (12)$$

¹¹The integration domain of the second summand is given by the hyperplane introduced due to the limitation $\delta\rho_{R_\omega}(-(p_1 + p_2 + p_3))$. We assume this to be covered in the measure $\bar{\mu}_{\overline{\Pi\Pi}}$ and do not discuss it explicitly, since for the one loop order the corresponding Lagrangian integral $\mathcal{L}_{f,\overline{\Pi\Pi},\mathcal{F}}$ vanishes.

The exponential now exactly represents the generating function $Z_{z,R_\omega}[J]$, such that the second moment against gaussian measure can be derived using two functional derivatives.

2.4.1 Theoretical Application of the Propagator Representation

Now the actual series expansion need to take place. It occurs in the definition of $\text{Ex}(\mathcal{L}_f)$, which can be expanded in its series form as

$$\text{Ex}(\mathcal{L}_f) = \text{id} + \mathcal{L}_f + \frac{1}{2} \cdot \mathcal{L}_f^2 + \sum_{n=3}^{\infty} \frac{1}{n!} \cdot \mathcal{L}_f^n.$$

Hereby we assign each component the names $n \mapsto \text{Ex}_n(\mathcal{L}_f)$. For the zeroth order we find ourselves an identity function, such that in the integral from equation (12) effectively only involves two functional derivatives, namely $\frac{\delta}{\delta \hat{J}(-x)}$ and $\frac{\delta}{\delta \hat{J}(-y)}$. Computation yields

$$\Delta_{\pm p}(Z_{z,R_\omega}^{(0)}[J]) = Z_{z,R_\omega}^{(0)}[J] \cdot \frac{\delta}{\delta \hat{J}(p)} \left(-\frac{1}{2} \cdot \int_{\mathbb{R}^d} G_0(q, z) \cdot \hat{J}(q) \delta_{-p}(dq) \right. \quad (13)$$

$$\left. -\frac{1}{2} \cdot \int_{\mathbb{R}^d} G_0(q, z) \cdot \hat{J}(-q) \delta_p(dq) \right) = G_0(p, z) \cdot Z_{z,R_\omega}^{(0)}[J]. \quad (14)$$

Lastly applying the evaluation $J = 0$ we obtain by normalization $Z_{z,R_\omega}^{(0)}[0] = 1$ the result $\Delta_{\pm p}(Z_{z,R_\omega}^{(0)}[J]) = G_0(p, z)$, which states the first Dyson summand. The following contributor corresponds to the first order of series expansion, i.e. $\text{Ex}_1(\mathcal{L}_f)$, in which the Lagrange operator initially appears. To begin with, the general form of $\mathcal{L}_{f,\mathcal{F}}$ reads

$$\begin{aligned} & \int_{(\mathbb{R}^d)^2} \mu_z(p) \cdot \left(\frac{\delta}{\delta \hat{J}(-p_1)} \circ \frac{\delta}{\delta \hat{J}(-p_1 - p_2)} \right) Z_{z,R_\omega}^{(0)}[J] \bar{\mu}_{\overline{\Pi}}(dp) \\ & \quad + \int_{(\mathbb{R}^d)^3} V_z(p_3, -p_2) \cdot \left(\frac{\delta}{\delta \hat{J}(-p_1)} \circ \frac{\delta}{\delta \hat{J}(-p_3)} \right) Z_{z,R_\omega}^{(0)}[J] \bar{\mu}_{\overline{\Pi}\overline{\Pi}}(dp). \end{aligned}$$

Without going any further, we For this scenario, we state that:

Lemma 2 (Vanishing third derivative of $Z_{z,R_\omega}^{(0)}$). For $p \in (\mathbb{R}^d)^3$ the composed directional derivatives of $Z_{z,R_\omega}^{(0)}[J]$ vanish, i.e. $\frac{\delta}{\delta \hat{J}(p_1)} \frac{\delta}{\delta \hat{J}(p_2)} \frac{\delta}{\delta \hat{J}(p_3)} Z_{z,R_\omega}^{(0)}[J] = 0$.

Proof. Let $Z_{z,R_\omega}^{(0)}[J]$ be defined as in 2.4, $\Delta_p := \frac{\delta}{\delta \hat{J}(p_1)} \frac{\delta}{\delta \hat{J}(p_2)} \frac{\delta}{\delta \hat{J}(p_3)}$ and $\frac{\delta}{\delta \hat{J}(\xi)} Z_{z,R_\omega}^{(0)}[J] = G_0(\xi, z) \cdot \hat{J}(-\xi) \cdot Z_{z,R_\omega}^{(0)}[J]$, then we can directly calculate the first directional derivative as

$$\Delta_p Z_{z,R_\omega}^{(0)}[J] = \frac{\delta}{\delta \hat{J}(p_1)} \frac{\delta}{\delta \hat{J}(p_2)} N_z^{(0)} \cdot (G_0(p_3, z) \cdot \hat{J}(-p_3)) \cdot Z_{z,R_\omega}^{(0)}[J].$$

Following the product rule and using the invariance of $N_z^{(0)}$ in respect to J we obtain

$$\begin{aligned}\Delta_p Z_{z,R_\omega}^{(0)}[J] &= N_z^{(0)} \cdot \frac{\delta}{\delta \hat{J}(p_1)} (G_0(p_3, z) \cdot \delta(-p_1 - p_2) \cdot Z_{z,R_\omega}^{(0)}[J] \\ &\quad + G_0(p_3, z) \cdot \hat{J}(-p_3) \cdot G_0(p_2, z) \cdot \hat{J}(-p_2) \cdot Z_{z,R_\omega}^{(0)}[J]).\end{aligned}$$

The last directional derivative gives us for the first summand

$$G_0(p_3, z) \cdot \delta(-p_1 - p_2) \cdot G_0(p_1, z) \cdot \hat{J}(-p_1) \cdot Z_{z,R_\omega}^{(0)}[J],$$

which vanishes for $J = 0$. The second summand again uses the product to yield three individual terms, which again all vanish for $J = 0$. q.e.d.

With the lemma we can safely assume that the first approximation order vanishes for $J = 0$ and therefore the second order is the first non-vanishing term in our approximation. This behaviour in uneven moments can be observed in a generalizing manner: For so called *centeralized gaussian vectors* X the following theorem of Isserlis/Wick holds.

Theorem 2.2. Isserlis'/Wick's Theorem.

Let $X : [N] \rightarrow (\Omega \rightarrow \mathbb{R}^d)$ be a random variable vector on $(\Omega, \mathcal{A}, \mathbb{P})$ with $\mathbb{E}(X_i) = 0$ for all $i \in [N]$. Let furthermore be $\mathbb{P} \gg \lambda^d$ with normal distribution f_Σ , then it holds that

$$\mathbb{E}\left(\prod_{i \in [N]} X_i\right) = \sum_{p \in P_N^2} \prod_{(i,j) \in p} \mathbb{E}(X_i \cdot X_j),$$

in which $P_N := \{M \subset \mathcal{P}([N]) : \#M = 2 \& \bigcup M = [N]\}$ is the set of all pair partitions to $[N]$.

Proof. The proof uses the concept of generating functions and can be found in [13]. q.e.d.

From the theorem it directly follows that for $N \in \text{uneven}$ we have an empty sum over P_N^2 and therefore the expectation value vanishes. We have to consider that Isserlis' theorem is only applicable for *normally distributed* random variables!

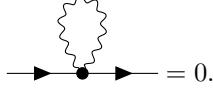
2.4.2 Visualization: Calculation of one One-Loop Correction Integral

We have already discussed the zeroth and first order of our operator series to $\text{Ex}(\mathcal{L}_{f,\mathcal{F}})$. The next order utilizes the third order operator $\text{Ex}_2(\mathcal{L}_f)$ to calculate the correlation of six total fluctuations Φ . This operator explicitly is of the form $\text{Ex}_2(\mathcal{L}_{f,\mathcal{F}}) = (\mathcal{L}_{f,\mathcal{F}})^2/2$. We therefore have to calculate the expression

$$\langle \Phi(\tilde{p}) \Phi(-\tilde{p}) \rangle_{\mathbb{G}_{\tilde{U},z,R_\omega}} \approx (\Delta_{\pm \tilde{p}} \circ \text{Ex}_2(\mathcal{L}_{f,\mathcal{F}})) Z_{z,R_\omega}^{(0)}[J] = \frac{1}{2} \cdot \Delta_{\pm \tilde{p}} (\mathcal{L}_{f,\mathcal{F},\bar{\Pi}}^2(Z_{z,R_\omega}^{(0)}))[J].$$

using $\Delta_{\pm\tilde{p}} := \frac{\delta}{\delta J(-\tilde{p})} \circ \frac{\delta}{\delta J(\tilde{p})}$. There are now three steps to be accomplished: (i) the discussion of the operator $\mathcal{L}_{f,\mathcal{F}}^2$, (ii) the evaluation of the correlator regarding the gaussian measure $\mathbb{G}_{\tilde{U},z,R_\omega}$ and (iii) the evaluation of the expectancy regarding the positional probability measure $\bar{\mu}_{\bar{\Pi}}$.

Starting with (i), notice how we have neglected the functional terms with $\mathcal{L}_{f,\mathcal{F},\bar{\Pi}\bar{\Pi}}$. This is due to the nature of *tadpoles*, which in one loop order are not contributing to the summation. The occurring vertex describes four connections, but for only one loop allowed the only diagram that could be thought of is



This allows us to neglect the second summand and focus on the first one. [3, 4] With its definition we find

$$\Delta_{\pm\tilde{p}} \left(\int_{(\mathbb{R}^d)^2} \mu_z(p) \cdot \left(\frac{\delta}{\delta J(-p_1)} \circ \frac{\delta}{\delta J(p_1 + p_2)} \right) \bar{\mu}_{\bar{\Pi}}(dp) \right)^2 Z_{z,R_\omega}^{(0)}[J].$$

Evaluation now goes twofold: First we have to process the four functional differential operators acting on the functional $J \mapsto Z_{z,R_\omega}^{(0)}[J]$. Second we need to turn off the external virtual fields J by evaluating at $J = 0$. The first substep then yields

$$\iint_{(\mathbb{R}^d)^2} \left[\int_{\mathcal{F}_{d,N}} \mu_z(p) \Phi(p_1) \Phi(-p_1 - p_2) \Phi(q_1) \Phi(-q_1 - q_2) \mu_z(q) \mathbb{G}_{\tilde{U},z,R_\omega}(d\Phi) \right] Z_{z,R_\omega}^{(0)}[J] d(p,q)$$

with $\iint = \int_{(\mathbb{R}^d)^2} \int_{(\mathbb{R}^d)^2}$ and measure $\bar{\mu}_{\bar{\Pi}}^2 = ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})^2 \cdot (2\pi)^{-4 \cdot d}$. The last functional derivatives involve the evaluation of $\Delta_{\pm\tilde{p}}$ which yet again yields two factors $\Phi(\tilde{p})$ and $\Phi(-\tilde{p})$ into the integrand's product. As this get visually challenging to read, we quickly evaluate $J = 0$ as no differentials are left to be evaluated, which by normalization results in $Z_{z,R_\omega}^{(0)}[J] = 1$.

See how we are now already at step (ii), since a gaussian correlator can be recognized due to the functional integral:

$$\iint_{(\mathbb{R}^d)^2} \mu_z(p) \cdot \mu_z(q) \cdot \langle \Phi(\tilde{p}) \cdot \Phi(p_1) \cdot \Phi(-p_1 - p_2) \cdot \Phi(q_1) \cdot \Phi(-q_1 - q_2) \cdot \Phi(-\tilde{p}) \rangle_{\mathbb{G}_{\tilde{U},z,R_\omega}} (\bar{\mu}_{\bar{\Pi}})^2(d(p,q)).$$

On this expected value we can use Isserlis'/Wick's theorem 2.2, since it is normally distributed:

$$\langle \Phi(x_1) \cdot \Phi(x_2) \cdot \Phi(-x_2 - x_3) \cdot \Phi(x_4) \cdot \Phi(-x_4 - x_5) \cdot \Phi(x_6) \rangle_{\mathbb{G}_{\tilde{U},z,R_\omega}} = \sum_{p \in P_6^2} \prod_{(i,j) \in p} \langle \Phi(x_i) \Phi(x_j) \rangle_{\mathbb{G}_{\tilde{U},z,R_\omega}}.$$

On this we can cleverly neglect

- (a) All terms in which the external fields $\Phi(\pm\tilde{p})$ are not connected to one internal pair $\Phi(p_1) \Phi(-p_1 - p_2)$ and $\Phi(q_1) \Phi(-q_1 - q_2)$ each.
- (b) All terms that yield the same value for the correct contraction of the external fields, i.e. the same value as the product over the partition p_0 yields. Since we sum over same values,

we can introduce a correction of $1/n$ with n being the number of equal terms.

The only non-vanishing term is the one with $p_0 = \{(p, p_1), (-p_1 - p_2, q_1), (-q_1 - q_2, -\tilde{p})\}$. The amount of equal terms is 8, where their value can be obtained by the following proposed contraction:

$$\underbrace{\langle \Phi(\tilde{p}) \Phi(p_1) \Phi(-p_1 - p_2) \Phi(q_1) \Phi(-q_1 - q_2) \Phi(-\tilde{p}) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}}}_{\text{inner part of the correlator}}$$

This leads to the simplification

$$\sum_{p \in P_6^2} \prod_{(i,j) \in p} \langle \Phi(x_i) \Phi(x_j) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}} \stackrel{(a),(b)}{=} 8 \cdot \prod_{y \in p_0} \langle \Phi(y_1) \cdot \Phi(y_2) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}} \quad (15)$$

where the product on the right hand side is given by the contraction above. With respect to our starting point we now found

$$\langle \Phi(\tilde{p}) \cdot \Phi(-\tilde{p}) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}} = \frac{1}{4} \cdot \iint_{(\mathbb{R}^d)^2} \prod_{(i,j) \in p_0} \langle \Phi(x_i) \Phi(x_j) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}} \cdot \mu_z(p) \cdot \mu_z(q) (\bar{\mu}_{\Pi})^2(d(p, q)).$$

Since we have already shown in the computation in equation (14) that the two point correlator yields $\langle \Phi(\xi) \Phi(\chi) \rangle_{\mathbb{G}_{\tilde{U}, z, R_\omega}} = G_0(\xi, z) \cdot \delta(\xi + \chi)$ for $\xi, \chi \in \mathbb{R}^d$, we can gather all restrictions to the integration domain introduced by each factor in the product of equation (15). This leads to the following restrictions regarding the integration domain $(\mathbb{R}^d)^2 \times (\mathbb{R}^d)^2$:

$$\begin{aligned} m(\tilde{p}) := & \{(p, q) \in (\mathbb{R}^d)^2 \times (\mathbb{R}^d)^2 : \tilde{p} + p_1 = 0\} \\ & \cap \{(p, q) \in (\mathbb{R}^d)^2 \times (\mathbb{R}^d)^2 : q_1 - p_1 - p_2 = 0\} \\ & \cap \{(p, q) \in (\mathbb{R}^d)^2 \times (\mathbb{R}^d)^2 : \tilde{p} + p_1 + p_2 = 0\}, \end{aligned}$$

Where the intersection operand \cap is used to formulate a logical AND. With this the double integral is equal to

$$\frac{1}{4} \cdot \iint_{m((\tilde{p}))} \mu_z(p) \cdot \mu_z(q) \cdot G_0(\tilde{p}, z)^2 \cdot G_0(q_1, z) (\bar{\mu}_{\Pi})^2(d(p, q)).$$

By the measure $\bar{\mu}_{\Pi}^2 = ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})^2 \cdot (2\pi)^{-4 \cdot d}$ we get another restriction to $\delta(x_2 + x_4)$, since a product of dirac measures occurs, which in notation of distributions using convolution leads to

$$\begin{aligned} \mathbb{E}(\rho_{R_\omega}(x_1) \cdot \rho_{R_\omega}(x_2)) &= \frac{1}{\rho_*^2} \cdot \sum_{m,n \in [N]} \int_{V_{d,N}} \delta_{\mathbf{r}_m}(x_1) \cdot \delta_{\mathbf{r}_n}(x_2) \cdot P(\mathbf{r}) \chi_R(d\mathbf{r}) \\ &= \frac{N \cdot (N-1)}{\rho_*^2 \cdot |V_{d,N}|^2} + \frac{N}{|V_{d,N}| \cdot \rho_*^2} \cdot \delta(x - y) \end{aligned}$$

and using the field shift $\rho_{R_\omega} = \square_{R_\omega} + \delta\rho_{R_\omega}$ finally $\mathbb{E}(\rho_{R_\omega}(x_1) \cdot \rho_{R_\omega}(x_2)) = \overline{\rho_{R_\omega}(x_1) \cdot \rho_{R_\omega}(x_2)} = \delta(x_1 - x_2)/\rho_*$ [3, 4]. Implementing this into the integration domain according to $M(\tilde{p}) :=$

$m \cap \{(p, q) \in (\mathbb{R}^d)^2 \times (\mathbb{R}^d)^2 : p_2 + q_2 = 0\}$ allows us to conclude the integral to

$$\int_{M(\tilde{p})} \mu_z(p_1, p_2) \cdot \mu_z(p_3, p_4) \cdot (G_0(\tilde{p}, z)^2 \cdot G_0(p_1, z)) \lambda(dp).$$

At this point we do not discuss if $M(\tilde{p})$ is a λ -null set and stay with the physical idea of conservation of momentum. Taking another closer look at $M(\tilde{p})$ lets us find a parametrization of our integration domain, such that we can transform the integral into one dimension. For this we only need to solve the following system of linear equations:

$$\begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & -1 & -1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \tilde{p} \\ p_1 \\ p_2 \\ q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

The solution to fixed \tilde{p} reduces to one variable q_1 and the following parametrizations:

$$p_1(q_1) = -q_1, \quad p_2(q_1) = \tilde{p} + q_1, \quad q_2(q_1) = -\tilde{p} - q_1.$$

With this we are equipped to transform the integral while renaming q_1 to q :

$$\frac{1}{\rho_*} \cdot G_0(\tilde{p}, z)^2 \cdot \int_{\mathbb{R}^d} G_0(q, z) \cdot \mu_z(-\tilde{p}, q + \tilde{p}) \cdot \mu_z(q, -q - \tilde{p}) \lambda(dq). \quad (16)$$

Using symmetry of μ_z regarding $\mu_z(-\tilde{p}, q - p) = \mu_z(q, -q - \tilde{p})$ and a linear shift $q \mapsto q - \tilde{p}$ we find

$$\frac{1}{\rho_*} \cdot G_0(\tilde{p}, z)^2 \cdot \int_{\mathbb{R}^d} G_0(q - \tilde{p}, z) \cdot \mu_z(\tilde{p}, -q)^2 \lambda(dq).$$

Since one can see the amount of consideration needed to evaluate every single integral into readable form, we move on to a much neater way of displaying the results in the following section.

2.5 Feynman Diagrammatics

While we have calculated the exact integrals occurring in the series expansion, for the human eye it is more appealing to visualize what is happening. This is where the *Feynman diagrammatics* come into play. They represent occurring integrals in form of *graphs*. They also allow an argumentation that not *all* diagrams are needed to represent the MGF, but only the *connected* ones [12, Sec. 4.3]. This can be seen by the following consideration.

2.5.1 Connected Diagrams

With a basic understanding of graphs we can now take a look at the Feynman diagrams and ask ourselves how we can represent the MGF using only *connected* graphs. From a top down perspective we can already claim the existence of a *disjunct separation* of Graphs occurring in the MGF-Summation. Let \mathcal{G} be the set of *all* graphs contributing to $Z_{z,r_\omega}[J]$, then we can

symbolically write the *sum over all diagrams* $D \in \mathcal{G}$ as¹²

$$Z_{z,r_\omega}[J] \propto \sum_{D \in \mathcal{G}} D.$$

To understand how we should deal with the summands D we can remember that each element in \mathcal{G} essentially represents some specific integral, which itself yields a number in \mathbb{R} . From this we can conclude $D \in \mathbb{R}$ and therefore use regular arithmetic operations on the graphs. If we now find without looking any closer at \mathcal{G} a representation of D in terms of *connected* graphs, we can use this expression to achieve our initial goal. The idea is the constructability of every graph $G \in \mathcal{G}$ from a basis of connected (or irreducible) graphs $C \in \mathcal{G}_c$. This follows from initial assumptions on the underlying hamiltonian of our system. With this and the mathematical interpretation of *construction* we can write

$$Z_{z,r_\omega}[J] \propto \sum_{D \in \mathcal{G}} \left(\frac{1}{s(D)} \prod_{C \in \mathcal{G}_c} C^{n(D)} \right).$$

Notice that we have defined an adequate function $n : \mathcal{G} \rightarrow \mathbb{N}$ which maps a graph to the number of required connections from one single $C \in \mathcal{G}_c$ to contribute to D . The factor $s : \mathcal{G} \rightarrow \mathbb{N}$ is furthermore a normalization since we assume the commutativity of the union operation and we do not want to count the same graph multiple times. Following this idea we get $s(D) = n(D)!$ and therefore

$$Z_{z,r_\omega}[J] \propto \sum_{D \in \mathcal{G}} \left(\frac{1}{n(D)!} \prod_{C \in \mathcal{G}_c} C^{n(D)} \right) = \prod_{C \in \mathcal{G}_c} \sum_{D \in \mathcal{G}} \frac{1}{n(D)!} C^{n(D)} = \exp \left(\sum_{C \in \mathcal{G}_c} C \right).$$

where the last equation can be seen as an exponential function for infinite groups of \mathcal{G} [11]. From another standpoint this founding lemma can be retrieved from graph theory:

Lemma 3 (Relation of Connected and Disconnected Representation [12]). Let \mathcal{G}_c be a set of distinct, connected and irreducible^a diagrams. Let furthermore \mathcal{G} be the set of all $C \in \mathcal{G}_c$ and all possible products of graphs in \mathcal{G}_c . Then it holds

$$\text{FunctionSum}(\mathcal{G}) = \exp(\text{FunctionSum}(\mathcal{G}_c)) - 1$$

where *FunctionSum* represents the function that by summarization of diagrams is composed, for example a relation to the MGF.

^aBy *irreducible* we mean $\forall C \in \mathcal{G}_c : \#C_1, C_2 \in \mathcal{G}_c : C_1 \cdot C_2 = C$, with \cdot stating a canonical product of two diagrams.

The proof can be found also found in Lemma 1 from [12]. Furthermore it closes the connection to the normalization constant of the MGF basis that we have found earlier in C.2.4, since neglecting the disconnected diagrams means their sum representing said constant entirely. This

¹²For our matter it is sufficient to consider the proportionality of the MGF. Lemma 3 states an equality that is related to this proportionality, but not further discussed since its purpose is already fulfilled. See for example *Goldstone's Theorem*.

therefore is an equivalent argument to the initial value of $Z_{z,r_\omega}[0] = 1$.

2.5.2 Diagrammatical Notation

The next step is to define the *symbols* used to represent different integral components. While technically this can be done by arbitrarily chosen drawings, it turns out that the systematic approach of *Feynman rules* is more useful and also includes a physical interpretation. As a starting point we define the *propagator*. It represents the free particle propagating from one point to another.

Definition 2.24. Diagrammatical Propagator.

We define the *diagrammatical propagator* symbol as

$$\longrightarrow := G_0(p, z)/\rho_*$$

for given $p \in \mathbb{R}^d$ and $z \in \mathbb{C}$ at a density $\rho_* \in \mathbb{R}$.

Since in scattering events a density fluctuation is created, we also need to define the *density fluctuation* as a symbol.

Definition 2.25. Diagrammatical Density Fluctuation.

We define the *diagrammatical density fluctuation* symbol as

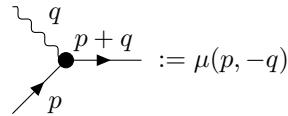
$$\sim\sim\sim := \mathbb{E}((\mathcal{F}\delta\rho_R)(q) \cdot (\mathcal{F}\delta\rho_R)(-q))/\rho_*$$

for given $\rho_* \in \mathbb{R}$ and a wave vector $q \in \mathbb{R}^d$ regarding the probability space $(\Omega, \mathcal{A}, \mathbb{P})$.

Considering scattering events, the first explicitly occurring one is notationally described by the three-point vertex μ_z . Its symbol should include an incoming particle, as well as an outgoing density fluctuation and a scattered particle.

Definition 2.26. Diagrammatical Three-Point Interaction.

We define the *diagrammatical three-point interaction* symbol as

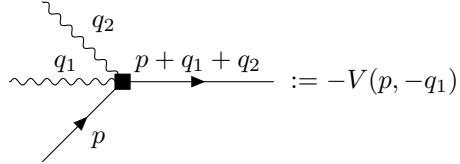


for given $p, q \in \mathbb{R}^d$, where the first argument describes the incoming mode and the second one the occurring density fluctuation.

Lastly the four-point interaction includes two particles and two density fluctuations.

Definition 2.27. Diagrammatical Four-Point Interaction.

We define the *diagrammatical four-point interaction* symbol as



for given $p, q_1, q_2 \in \mathbb{R}^d$, where the first argument describes the incoming mode and the second one of the density fluctuations.

All definitions now correspond to literatures conventions, see [3, 4]. Having these notations defined we can take a second look at integral 16 to obtain the following diagrammatical representation:

$$\text{Diagram with two horizontal lines and a loop above them} = \frac{1}{\rho_*} \cdot G_0(\tilde{p}, z)^2 \cdot \int_{\mathbb{R}^d} G_0(q - \tilde{p}, z) \cdot \mu_z(\tilde{p}, -q)^2 \lambda(dq). \quad (17)$$

It is now much easier to think about other integrals that can occur in one loop order, since a visual representation is given. Another way of having one loop is to neglect one of the propagators in the diagram above, namely the first. This yields the following diagram, from which the integral form can be derived using the stated Feynman rules.

$$\text{Diagram with one horizontal line and a loop above it} = -\frac{2}{\rho_*} \cdot G_0(\tilde{p}, z) \cdot \int_{\mathbb{R}^d} G_0(\tilde{p} - q, z) \cdot \mu_z(\tilde{p}, -q) \lambda(dq), \quad (18)$$

The last possibility without loosing connectiveness is to neglect the second propagator. This yields the following diagram.

$$\text{Diagram with one horizontal line and a loop above it} = \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(\tilde{p} - q, z) \lambda(dq). \quad (19)$$

These diagrams exactly match the literature's results [3] and state our final theoretical standpoint for starting the position probability correction. In addition, performing a summation closes the loop and gives the first order self energy: Calling $L_i^{(1)}$ the i -th diagram in one loop order, we have

$$\begin{aligned} \sum_{i \in [3]} L_i^{(1)} &= \frac{G_0(p, z)}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \cdot \mu_z(p, -q)^2 \lambda(dq) \\ &\quad - 2 \cdot \frac{G_0(p, z)^2}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \cdot \mu_z(p, -q) \lambda(dq) \\ &\quad + \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \lambda(dq). \end{aligned} \quad (20)$$

Combining all three integrands into one we further find

$$\begin{aligned} \sum_{i \in [3]} L_i^{(1)} &= \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \cdot (G_0(p, z)^2 \cdot \mu(p, -q)^2 - 2 \cdot G_0(p, z) \cdot \mu(p, -q) + 1) \lambda(dq) \\ &= \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \cdot (G_0(p, z) \cdot \mu(p, -q) - 1)^2 \lambda(dq). \end{aligned}$$

With theorem and definitions 2.2 and 2.3 we can rewrite the content of the brackets using the vertex function:

$$G_0 \cdot \mu = G_0 \cdot G_0^{-1} + G_0 \cdot V = 1 + G_0 \cdot V \iff G_0 \cdot \mu - 1 = G_0 \cdot V. \quad (21)$$

This results in the dyson representation and self energy term

$$\sum_{i \in [3]} L_i^{(1)} = G_0(p, z)^2 \cdot \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} G_0(p - q, z) \cdot V(q, p)^2 dq =: G_0(p, z)^2 \cdot \Sigma^{(1)}(p, z).$$

2.6 Dyson Fixed Point Equation

To conclude the investigation led by the last few sections, we combine the gained intuition and formalisms within the *Dyson Fixed Point Equation*. As we have seen, diagrams produced by the perturbative ansatz lead to a large amount of integrals that should be ordered to be interpreted more easily. This can be done by gathering all diagrams with the same loop count and build their sum:

$$G = L^0 + \sum_{i \in [3]} L_i^{(1)} + \sum_{i \in [18]} L_i^{(2)} + \dots$$

Within this representation we have discussed the first two summands. As in the derivation of the one loop diagrams already shown, each sum can be disassembled into a product of the *bare propagator* G_0 and a *self energy* term corresponding to the loop count. Following the last chapter and [3, 4] we therefore have

$$G = G_0 + G_0^2 \cdot \Sigma^{(1)} + G_0^3 \cdot (\Sigma^{(2)})^2 + \dots = G_0 + \sum_{i=1}^{\infty} G_0^{i+1} \cdot (\Sigma^{(i)})^i.$$

Pulling out one bare propagator G_0 from the sum we can rewrite the equation as

$$G = G_0 + G_0 \cdot \sum_{i=1}^{\infty} (G_0 \cdot \Sigma^{(i)})^i = G_0 \cdot \sum_{i=0}^{\infty} (G_0 \cdot \Sigma^{(i)})^i.$$

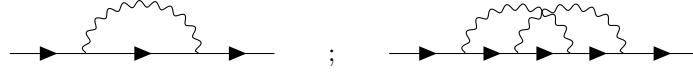
With $\Sigma^{(i)} = \Sigma^{(j)}$ for $i \neq j$ being now called simply Σ we would now be able to write for $G_0 \cdot \Sigma \in [0, 1)$ the geometric series

$$\sum_{i=0}^{\infty} (G_0 \cdot \Sigma)^i = \frac{1}{1 - G_0 \cdot \Sigma}.$$

From which the dyson equation can be derived as

$$G = \frac{G_0}{1 - \Sigma \cdot G_0} \iff G = G_0 + G_0 \cdot \Sigma \cdot G.$$

But this step needs a bit of clarification, as it involves a physical meaning. Looking at the Feynman diagrams occurring in the summation, they all share a similar starting and ending configuration, which can be seen in the first two loop orders by example:



Notice that every diagram has equal incoming and outgoing wave vectors p and different internal scattering events inbetween. Since we sum up all diagrams we, in physical terms, consider all possible scattering events that can occur within a certain loop order, which means effectively an equality of all $\Sigma^{(i)}$ externally. With this we can state the fixed point equation.

Definition 2.28. Dyson Fixpoint Equation.

For $G_0 \in \mathbb{R}$ and $\Sigma \in \mathbb{R}$, the propagator G is under the condition $G_0 \cdot \Sigma \in [0, 1)$ given by the Dyson Fixpoint Equation

$$G = G_0 + G_0 \cdot \Sigma \cdot G \iff G = \frac{1}{G_0^{-1} - \Sigma}.$$

Hereby G_0 states the system's bare propagator and Σ the self energy term.

↪ DENSITY FLUCTUATION ANALYSIS ↵

Chapter 3

Up until now we have been discussing uncorrelated systems of particles, in which the probability of particle occurrence is given without consideration of other particles positions. This simplification is not applicable due to several caveats, such as the vanishing probability in the large volume limit $|V_{d,N}| \rightarrow \infty \implies 1/|V_{d,N}| \rightarrow 0$ and no consideration of the medium's *structure* in any way. We aim to introduce this property into the formalism and to present an approximation for higher order diagrams in the Dyson expansion.

3.1 Expectancy of Density Fluctuation

Connecting to our previous sections, due to $P(r) = 1/|V_{d,N}|$ in our earlier theory we could evaluate

$$\begin{aligned}\mathbb{E}_\omega(\rho_{R_\omega}(x)) &= \int_{V_{d,N}} \frac{1}{\rho_*} \cdot \sum_{n \in [N]} \delta_y(x) (P \cdot \lambda_R)(dy) \\ &= \frac{1}{\rho_*} \cdot \sum_{n \in [N]} \int_{V_{d,N}} \delta_0(x) \cdot P(x - y) \lambda_R(dy) \\ &= \frac{1}{\rho_*} \cdot \sum_{n \in [N]} (\delta * P)(x) = \frac{1}{\rho_*} \cdot \sum_{n \in [N]} \delta(P(x - \cdot)) = 1.\end{aligned}$$

This result is not surprising, since we have defined the density measure as a normalized sum of δ distributions. The introduction of the *change of measures* in Definition 2.21 established $\rho_{R_\omega} = \square_{R_\omega} + \delta\rho_{R_\omega}$, which in this case concludes to $\mathbb{E}(\delta\rho_{R_\omega}(x)) = 0$. Applying the Fourier transform to both sides results in the same conclusion considering linearity of operations: $(\mathcal{F} \circ \mathbb{E}_\omega)(\delta\rho_{R_\omega})(q) = \int_{V_{d,N}} \mathcal{F}(\delta\rho_{R_\omega})(q) \mathbb{P}(d\omega) = 0$. Remaining a Fourier perspective opens us the door to the structure factor $S_*(q)$, which we are introducing as

$$\mathbb{E}_\omega((\mathcal{F}\delta\rho_{R_\omega})(q) \cdot (\mathcal{F}\delta\rho_{R_\omega})(-q)) = S_*(q) - 1.$$

following [14]. This can be immediately deduced from definition using integral linearity:

$$\mathbb{E}_\omega(\hat{\delta\rho}_{R_\omega}(q) \cdot \hat{\delta\rho}_{R_\omega}(-q)) = \mathbb{E}_\omega((\hat{\rho}_{R_\omega}(q) - 1) \cdot (\hat{\rho}_{R_\omega}(-q) - 1)) = \mathbb{E}_\omega(\hat{\rho}_{R_\omega}(q) \cdot \hat{\rho}_{R_\omega}(-q)) - 1.$$

Explicitly writing Fourier transformed functional of ρ_{R_ω} , which can be proven to be $\hat{\rho}_{R_\omega}(q) = \sum_{i \in [N]} \exp(-\hat{i} \cdot \langle q, R_\omega(i) \rangle)/\rho_*$ using C.2.1, the definition again yields

$$\mathbb{E}_\omega(\rho_{R_\omega}(q) \cdot \rho_{R_\omega}(-q)) = \frac{1}{\rho_*^2} \cdot \mathbb{E}_\omega \left(\sum_{(i,j) \in [N]^2} \exp(-\hat{i} \cdot \langle q, R_\omega(i) \rangle) \cdot \exp(\hat{i} \cdot \langle q, R_\omega(j) \rangle) \right). \quad (22)$$

The sum can now be manipulated such that we get the relation to the radial distribution function $y \mapsto g_x(y)$ for given reference points $x \in \Gamma$:

Lemma 4 (Static Structure Factor and Radial Distribution Function). Let $S_*(q) := \mathbb{E}(\hat{\delta\rho}_r(q) \cdot \hat{\delta\rho}_r(-q))$ for $r \in (\Omega \mapsto \mathbb{R}^d)^N$ and $q \in \mathbb{R}^d$ be the static structure factor for the Fourier transformed density functional $\hat{\rho}_r(q) = \sum_{i \in [N]} \exp(-i \cdot \langle r, q \rangle) / \rho_*$. Then the static structure factor is given by

$$\mathbb{R}^d \ni q \mapsto S_*(q) = 1 + \rho_* \cdot (\mathcal{F}(g_0 - 1))(q).$$

The lemma also directly states that the structural properties of an isotropic liquid is strongly related to the Fourier transform of a radial distribution function g . Because we are interested in structural dependencies, this function g needs some further discussion before we can proceed with the lemma's proof.

3.1.1 The Particle Distribution Density

To start off, for the radially symmetric case we find that two particles $r_1, r_2 \in \Gamma$ lie within a given distance $x_* \in \mathbb{R}_{>0}$ when $r_1 - r_2 \in B_{x_*}(0)$, i.e. the difference vector being *at most* of certain length x_* . To have exactly distance x_* from each other further means $r_1 - r_2 \in \partial B_{x_*}(0)$, i.e. the difference being *exactly* of length x_* . This can be expressed for any direction $e \in \partial B_1(0)$ as $\delta(x_* \cdot e - (r_1 - r_2))$ or $\delta(x - (r_1 - r_2))$ for $x = x_* \cdot e$. If we now vary x_* within a given boundary $\varepsilon \in \mathbb{R}_{>0}$ we can compute the probability of finding particles $r_1, r_2 \in \Gamma$ within the annulus $B_{x_*, \varepsilon}(0) := B_{x_* + \varepsilon}(0) \setminus B_{\min(x_* - \varepsilon, 0)}(0)$ given by x_* and ε , i.e. being within distance $(x_* - \varepsilon, x_* + \varepsilon)$ from each other. Comparing all particles for a distribution $r \in V_{d,N}$ we can deduce the density for the system being in the state of pair distances $x_* \pm \varepsilon$ as the sum of all restrictions neglecting all self-comparisons (denoted by $[N]_{\neq}^2 := \{(i, j) \in [N]^2 : i \neq j\}$):

$$V_{d,n} \ni r \mapsto \sum_{(i,j) \in [N]_{\neq}^2} \delta(x_* \cdot e - (r_i - r_j)).$$

Expanding the restriction $x_* \cdot e - (r_i - r_j) = 0$ to $x_* \cdot e - r_i = -r_j \iff y + x_* \cdot e - r_i = y - r_j$ and varying over an artificial test position $y \in \Gamma$ gives us the equality

$$\delta(x_* \cdot e - (r_i - r_j)) = \int_{\Gamma} \delta(y + x_* \cdot e - r_i) \delta(y - r_j) \lambda(dy),$$

which yields under sum and integral interchangeability the result

$$\sum_{(i,j) \in [N]_{\neq}^2} \delta(x_* \cdot e - (r_i - r_j)) = \int_{\Gamma} \sum_{(i,j) \in [N]_{\neq}^2} \delta(y + x_* \cdot e - r_i) \delta(y - r_j) \lambda(dy).$$

Let us now illustrate this concept before further analysis using $N = 5 + 3$ particles in \mathbb{R}^2 with $x_* = 3$ and $\varepsilon = 0.5$, see figure 4.

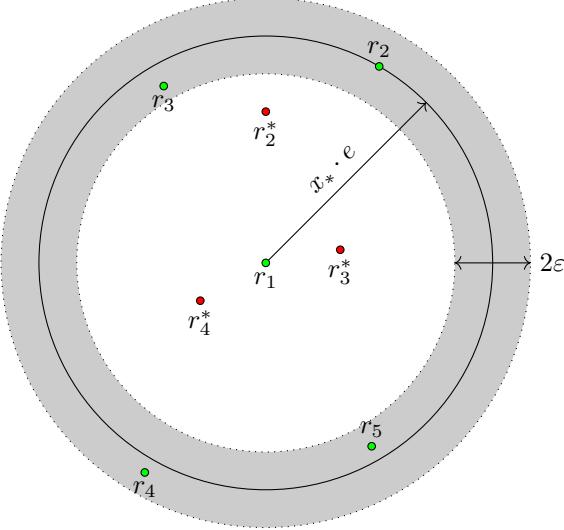


Figure 4: Visualization of the radial concept. In the center is the reference particle $r_1 \in \Gamma$, around which other particles are distributed. The red particles r_i^* are not fulfilling the condition $r_1 - r_i^* \in B_{x^*,\varepsilon}(0)$. The green particles r_i are fulfilling the condition. The illustration suggests that the probability of particles being within range x^* with r_1 is higher than the probability of particles being outside of this range.

A generalization of this concept can be found in [14] where the equilibrium n -particle distribution function is given via the hamiltonian H of our system, which can be reduced to only the first taylor approximation term $U(r)$ to define the n -particle density via D.3.29.

Definition 3.29. n Particle Density.

For our space of positions $\Gamma \subset \mathbb{R}^d$ from definition 2.13 we define the probability of finding n particles in a subvolume $U \subseteq \Gamma$ by its density

$$\Gamma^n \ni x \mapsto \rho_N^{(n)}(x) := C(N, n, h) \cdot \int_{V_{d,n-n} \times \text{TF}(V_{d,n-n}, x)} \exp(-\beta \cdot H(x, \phi)) \mathcal{D}(d(x, \phi)).$$

Within we use the abbreviation $C(N, 2, h) := \frac{N!}{(N-2)!} \cdot \frac{1}{h^{d \cdot N} \cdot N! \cdot 2!}$ for the normalization constant.^a

^aThe prefactor $C(N, n, h)$ is of combinatorial and physical nature, as it for example encodes interchangeability of particles by $1/N!$ and hereby suppressing paradoxes like the Gibbs paradox. Other factors like h assure continuity of the density and represent the planck constant in quantum mechanics. For further information see [12].

The occurring integral is also known in literature and statistical mechanics as a not fully integrated *partition function*, since the configuration space only applies to $n \leq N$ particles. For $r \in V_{d,n}$ with $n \in [N]$ we now again follow [14] where the particle distribution function is given by the n -particle density $\rho_N^{(n)}$ and a normalization to $\prod_{i \in [n]} \rho_N^{(1)}(r_i)$, i.e.

$$g_N^{(n)}(r) = \frac{\rho_N^{(n)}(r)}{\prod_{i \in [n]} \rho_N^{(1)}(r_i)}.$$

Looking at the $n = 2$ point correlation we have to consider two points $x_1, x_2 \in V_{d,N}$ within an ensemble of N particles. Formally we then have

$$g_N^2(x_1, x_2) \cdot (\rho_N^{(1)}(x_1) \cdot \rho_N^{(1)}(x_2)) = \rho_N^{(2)}(x_1, x_2). \quad (23)$$

If we now ask for the probability of finding a particle x_2 within a certain range $x_* \in \mathbb{R}_{>0}$ from a reference particle $x_1 \in \Gamma$ we can integrate over the annulus $B_{x_*, \varepsilon}(x_1)$ presented earlier to define

$$g_\varepsilon(x_1, x_*) := \int_{B_{x_*, \varepsilon}(x_1)} g_N^{(2)}(x_1, r) \lambda(dr).$$

which now can be connected to the structure factor $S_*(q)$. Its form can empirically be seen from an example in figure 5 or later on in our numerical results. Notice that for $x_1 = 0$ the function g_0 becomes the literature's radial distribution function [12].

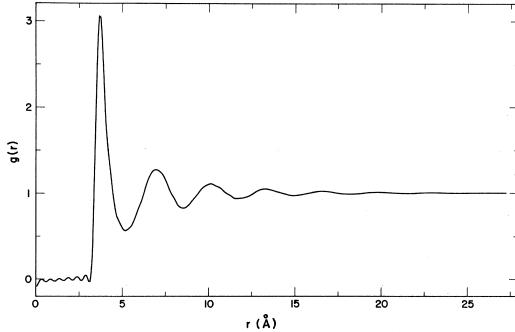


Figure 5: Example of a radial distribution function $g_{||}(x_*)$ for ^{36}Ar at a temperature of 85° from [15]. It can be seen that for specific lengths greater than 2.5\AA the radial distribution function jumps from nearly 0 to an amplitude above 3. Additionally an oscillating nature can be observed for all radii with different frequencies before and after the jump. For radii greater than 3\AA there can be specific maxima and minima localized in which the probabilities of finding a particle noticeably increase or decrease. Towards greater distances from the reference particle the function converges to 1, which physically indicates loss of structural information.

Lemma 5 (Expectancy of Two Restrictions). Let $x_1, x_2 \in \Gamma$ be two fixed points in the modelling space. Then for $C(N, 2, h) := \frac{N!}{(N-2)!} \cdot \frac{1}{h^{d \cdot N} \cdot N! \cdot 2!}$ and $M(N, 2) := \Gamma^{N-2} \times \text{TF}(\Gamma^{N-2}, r)$ we have

$$\langle \delta(x_1 - r_1) \cdot \delta(x_2 - r_2) \rangle_{P_r \cdot \lambda} = C(N, 2, h) \cdot \int_{M(N, 2)} \exp(-\beta \cdot H((x_1, x_2, r), \cdot)) \lambda(dr),$$

where $r \mapsto \exp(-\beta \cdot H(r, \cdot)) = P_r(r)$. Furthermore it holds from definition 3.29 that

$$\rho_N^{(2)}(x_1, x_2) = \left\langle \sum_{(i,j) \in [N]^2_{\neq}} \delta(x_1 - r_i) \cdot \delta(x_2 - r_j) \right\rangle_{P_2 \cdot \lambda}.$$

3.1.2 Relation to the Structure Factor

The introduction of the structure factor $S_*(\mathbf{q})$ enhances accessibility of the theory to experimental data, as it can be measured directly in scattering experiments, in particular in X-ray or neutron scattering [16]. This means measureability of the particle probability distribution. Recalling our result from lemma 4 we have been able to retrieve a connection between the structure factor $S_*(\mathbf{q})$ and the radial distribution function $g_0(\mathbf{x})$ following

$$\mathbb{R}^d \ni \mathbf{q} \mapsto S_*(\mathbf{q}) = 1 + \rho_* \cdot (\mathcal{F}(g_0 - 1))(\mathbf{q}).$$

Using $g_N^{(2)} = \rho_N^{(2)} / \rho_*^2$ and lemma 5 we can see the particle density function appearing in the structure factor:

$$\mathbb{E}(\rho_{R_\omega}(\mathbf{q}) \cdot \rho_{R_\omega}(-\mathbf{q})) = 1 + \rho_* \cdot \left[\mathcal{F}_x \left(\mathbf{x} \mapsto \frac{1}{\rho_*^2 N} \left\langle \sum_{(i,j) \in [N]^2 \neq} \delta(\mathbf{x} - \mathbf{r}_j + \mathbf{r}_i) \right\rangle_{P_r \cdot \lambda(d\mathbf{r})} \right) - 1 \right] (\mathbf{q}).$$

Hereby the used probability measure $P_r \cdot \lambda = \mathbb{P}_1$ is given by the particle density $P_r : V_{d,N} \ni R \mapsto \exp(-\beta \cdot U(R))$. Within the original Taylor expansion of U came into play, as it allows the detachment to the probability measure of ϕ given by $P_\phi \cdot \lambda = \mathbb{P}_2$. Expanding the definition gives a clearer picture of this structure:

$$\left\langle \sum_{(i,j) \in [N]^2 \neq} \delta(\mathbf{x} - \mathbf{r}_j + \mathbf{r}_i) \right\rangle_{P_r \cdot \lambda(d\mathbf{r})} = C_{N,2,h} \cdot \sum_{(i,j) \in [N]^2 \neq} \int_{V_{d,N}} \exp(-\beta \cdot U(\pi_{ij}(\mathbf{x}, \mathbf{r}))) \lambda(d\mathbf{r}).$$

The mapping π_{ij} can be interpreted as an iteration over all particle pair combinations where one particle is fixed at the origin and the other is shifted by the difference vector of the pair. Therefore we have tuples of vector entries in $V_{d,N}$ which can be displayed in a matrix form, where the diagonal entries are neglected due to summation specification:

$$\pi_{ij}(\mathbf{x}, \mathbf{r}) := \begin{pmatrix} (0, \mathbf{x}, \mathbf{r}_j, \dots, \mathbf{r}_N) & \dots & (0, \mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{x}) \\ (\mathbf{x}, 0, \mathbf{r}_3, \dots, \mathbf{r}_N) & \dots & (\mathbf{r}_1, 0, \mathbf{r}_2, \dots, \mathbf{x}) \\ \vdots & \vdots & \vdots \\ (\mathbf{x}, \mathbf{r}_2, \dots, \mathbf{r}_{N-1}, 0) & (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{x}, 0) & \dots \end{pmatrix}$$

To conclude this discovery, integral interchangeability allows us to drag the probability measure $P_r \cdot \lambda$ out of the expression to get

$$\begin{aligned} 1 + \rho_* \cdot \left[\mathcal{F}_x \left(\sum_{(i,j) \in [N]^2 \neq} \delta(r - \mathbf{r}_j + \mathbf{r}_i) \right)_{P_r \cdot \lambda(d\mathbf{r})} - 1 \right] (\mathbf{q}) \\ = 1 + \int_{V_{d,N}} \mathcal{F}_x \left(\frac{1}{\rho_*^2 N} \cdot \sum_{(i,j) \in [N]^2 \neq} \delta(r - \mathbf{r}_j + \mathbf{r}_i) \right) P_r \cdot \lambda(d\mathbf{r}). \end{aligned}$$

With these results the corrected probability measure \mathbb{P} can be written as $\mathbb{P} = P_r \cdot \lambda \otimes P_\phi \cdot \lambda =$

$(P_r \cdot P_\phi) \cdot \lambda^2$. It results in the following form for the resolvent G_N :

$$\int_{V_{d,N}} \int_{\text{TF}(V_{N,d})} (\Delta_{\pm p} \circ \text{Ex}_{\mathcal{L}_f}) \left(\underbrace{\exp(-\beta \cdot (U(r) + \langle \tilde{U}(f, r) \cdot \phi, \phi \rangle))}_{\text{for } P_r} \right) \underbrace{\lambda(dr) \lambda(d\phi)}_{\text{for } P_\phi}.$$

This now states the resolvent G_N in the corrected ERM model, where correlated disorder is taken into account. In a last step we want to verify Lemma 4 which gave the connection of the correlation function to the static structure factor by idea-proving it.

Idea of proof. We only discuss the proof idea here because for its full extent we have to consider distributions and their properties.

Following definitions we have established equation (22) which now can be transformed to the sum over non-diagonal elements plus the diagonal elements of the matrix $(i, j) \mapsto \exp(-\overset{\circ}{i} \cdot \langle q, r_i - r_j \rangle)$. Since for diagonal elements we have $(i, i) \mapsto 1$ and the sum reduces with $\mathbb{E}_\omega(\sum_{i \in [N]} 1) = N$ to

$$N \cdot S_*(q) = N + \mathbb{E}_r \left(\sum_{(i,j) \in [N]^2_{\neq}} \exp(-\overset{\circ}{i} \cdot \langle q, r_i - r_j \rangle) \right).$$

Introducing two dirac integrals over δ_{r_i} and δ_{r_j} we can further write the expected value as

$$\mathbb{E}_r \left(\sum_{(i,j) \in [N]^2_{\neq}} \int_{(\mathbb{R}^d)^2} \exp(-\overset{\circ}{i} \cdot \langle q, x_1 - x_2 \rangle) (\delta_{r_i} \otimes \delta_{r_j})(dx) \right).$$

Interchanging the expectation operator with the integral and using lemma 5 we can hide the sums per definition of the 2-particle density $\rho_N^{(2)}$ that will be introduced in definition 3.29 to obtain

$$N \cdot S_*(q) = N + \int_{(\mathbb{R}^d)^2} \exp(-\overset{\circ}{i} \cdot \langle q, x_1 - x_2 \rangle) (\rho_N^{(2)} \cdot (\delta_{r_1} \otimes \delta_{r_2}))(dx_1, dx_2).$$

Translation invariance then leads to the result

$$S_*(q) = 1 + \rho_* \cdot \int_{\mathbb{R}^d} \exp(-\overset{\circ}{i} \cdot \langle q, x \rangle) \cdot g_0(x) \lambda(dx).$$

Because of this being a distributional equality which experimentally is not accessible, we have to regularize the integrand by shifting g_0 by its limit $A := \lim_{x_* \rightarrow \infty} g_{||}(x, x_*) = 1$ to obtain the final result. \diamondsuit

Since diagrammatical description turned out to be a powerful tool in the analytical derivation of the series expansion for the Dyson formalism, we take a look at the corrected Feynman rules in the next section.

3.2 Structural Corrected Diagrammatics

Since our change in the ERM formalism explicitly happened in the density fluctuation correlation, we need to modify definition 2.25 to include the amplitude $S_*(q)$. This can be done by simply replacing the constant 1 with $S_*(q)$ in the definition. The new diagrammatical representation of the density fluctuation then reads:

Definition 3.30. Diagrammatical Density Fluctuation with Structural Characteristic.

We redefine, under consideration of the medium's structure, the *diagrammatical density fluctuation* as

$$\sim\sim\sim := S_*(q)/\rho_*$$

for given $\rho_* \in \mathbb{R}$ and a wave vector $q \in \mathbb{R}^d$. Hereby the amplitude $S_*(q)$ is given by $q \mapsto 1 + \rho_* \cdot (\mathcal{F}(g_0 - 1))(q)$ for a radial distribution function $g_0 : \mathbb{R}^d \rightarrow \mathbb{R}$.

To now apply the newly developed theory we aim to reproduce the diagrammatics produced in [3] and deduced in equations (16) through (16). Since the vertices have the same definition as before, we can directly use the Feynman rules to adjust the previous results in first loop order:



$$= \frac{1}{\rho_*} \cdot G_0(\tilde{p}, z)^2 \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(q - \tilde{p}, z) \cdot \mu_z(\tilde{p}, -q)^2 \lambda(dq), \quad (24)$$



$$= -\frac{2}{\rho_*} \cdot G_0(\tilde{p}, z) \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(\tilde{p} - q, z) \cdot \mu_z(\tilde{p}, -q) \lambda(dq), \quad (25)$$



$$= \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(\tilde{p} - q, z) \lambda(dq). \quad (26)$$

With knowledge of all contributing terms we can once more calculate the first order self energy by summation. Following equation (20) we find

$$\begin{aligned} \sum_{i \in [3]} L_i^{(1)} &= \frac{G_0(p, z)}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(p - q, z) \cdot \mu_z(p, -q)^2 \lambda(dq) \\ &\quad - 2 \cdot \frac{G_0(p, z)^2}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(p - q, z) \cdot \mu_z(p, -q) \lambda(dq) \\ &\quad + \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(p - q, z) \lambda(dq). \end{aligned}$$

Again using the relation $G_0 \cdot \mu - 1 = G_0 \cdot V$ from equation (21) we find the corrected first loop order self energy as

$$\sum_{i \in [3]} L_i^{(1)} = G_0(p, z)^2 \cdot \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(q) \cdot G_0(p - q, z) \cdot V(q, p)^2 \lambda(dq) =: G_0(p, z)^2 \cdot \Sigma_{S_*}^{(1)}(p, z).$$

Having accomplished the development of one loop theory with structural corrections implemented into the diagrammatics, we can state the dyson fixed point equation for this order as

$$G_N(p, z) = G_0(p, z) + G_0(p, z)^2 \cdot \Sigma_{S_*}^{(1)}(p, z) \cdot G_N(p, z).$$

This form can be iteratively solved numerically, which will be object of the last chapter.

3.2.1 Gaussian Probability Density Approximation

Since for one loop diagrams we encounter at max a combination of two $\delta\rho_{R_\omega}$ measures, we can simply take its average using the gained density $r_* \mapsto \exp(-\beta \cdot U(r_*))$. Looking at the two loop diagrams we have to do a bit of argumentation, since

$$(\text{Ex}_3(\mathcal{L}_f) Z_{z, R_\omega}^{(0)})[J] = \frac{1}{6} \cdot (\mathcal{L}_{f, mcF, \bar{\Pi}} + \mathcal{L}_{f, \mathcal{F}, \bar{\Pi}\bar{\Pi}})^3 Z_{z, R_\omega}^{(0)}[J]$$

yields the measure

$$((\square_{R_\omega}) \otimes \delta\rho_{R_\omega}) \otimes ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega}) \otimes ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega}).$$

As for the fourth order $(\text{Ex}_4(\mathcal{L}_f) Z_{z, R_\omega}^{(0)})[J]$ there appear four total $\delta\rho_{R_\omega}$ measures in the same product, and so on. Since there is an integration to be made over all $\omega \in \Omega$, i.e. $e^{-\beta \cdot H(r, \phi)} \cdot \lambda(d(r, \phi))$ with regard to the particle positions r , we need to eventually calculate

$$\int_{V_{d, N}} ((\square_{R_\omega}) \otimes \delta\rho_{R_\omega})^n \cdot (\exp(U) \cdot \lambda)(d(r_*)), \quad n > 2.$$

Because the mapping $r_* \mapsto e^{-\beta \cdot U(r_*)}$ is generally not of gaussian form $x \mapsto \exp(-\langle A \cdot x, x \rangle / 2)$, we need to perform an approximation that has not been necessary before for the apriori density $r_* \mapsto 1/|V_{d, N}|$. For this we refer to the work of Gavin E. Crooks and David Chandler in [17], which states for the hard sphere model that for medium densitys ρ_* the probability measure \mathbb{P}_N for $N \in \mathbb{N}$ particles has the approximative density function $x \mapsto \exp(-\langle A \cdot (x - \nu_{MC}), x - \nu_{MC} \rangle / (2 \cdot \sigma_{MC}))$, where ν_{MC} and σ_{MC} respectively are expected values and standard deviations of a Monte Carlo simulation. Hereby we suggest making an error by approximation of the correct density $r_* \mapsto \exp(-\beta \cdot U(r_*))$ with a gaussian density:

$$\exp(-\beta \cdot U(r_*)) \approx \exp(-\langle A \cdot (r_* - \nu_{MC}), r_* - \nu_{MC} \rangle / (2 \cdot \sigma_{MC})),$$

This means that the theorem of Isserlis/Wick can be applied to the probability density of particle positions and our result $\hat{\delta\rho}_{R_\omega}(q) \cdot \hat{\delta\rho}_{R_\omega}(-q) = S_*(q)/\rho_*$ can be applied. Figure 6 shows in subfigure 6a the values of $\mathbb{P}_N(V)$ for various diameters 2.0σ to 4.0σ at a fixed density of 0.5. It can be seen that for all diameters the distribution nearly follows a gaussian form. The diameter 2.0σ furthermore corresponds to the exclusion volume of the hard sphere model, i.e. the volume in which no other particle can be found. On the other hand, the largest volume 4.0σ is 64 times as large as that of one particle. Subfigure 6b varies the density from 0.1 to 0.9 at a fixed volume diameter of 3.5σ . One can clearly see deviations for high and low densities from the gaussian form [17].

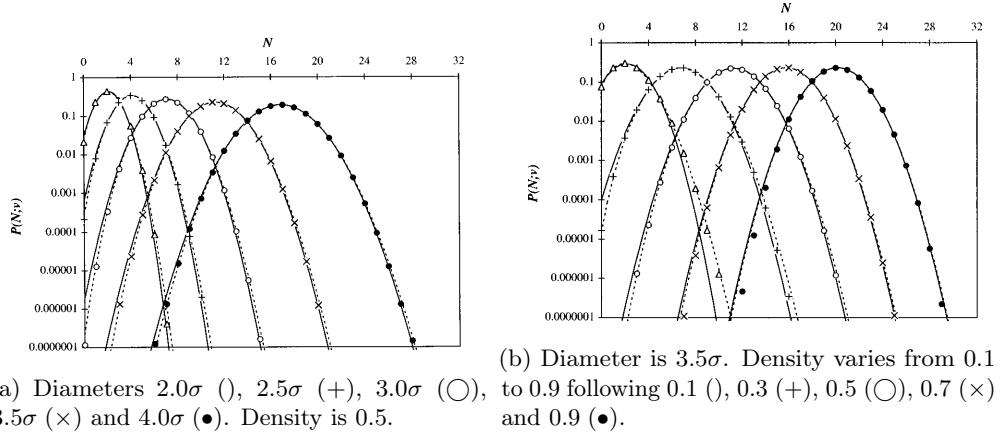


Figure 6: Values of $\mathbb{P}_N(V)$ for spherical volumes V_σ for finding N particles within. The points were gained by computer simulation, lines follow a gaussian distribution.

3.2.2 Relation to other Correlation Approaches

As we have mentioned in the beginning, there was another approach made towards the implementation of correlated disorder into the ERM model by Martin-Mayor in [5]. In chapter IV of his work he introduces a method to implement a Gibbs distribution (in our wording also known as Boltzmann distribution) into the ERM model. It is achieved by multiplication with the corresponding measure, in our case the Lebesgue measure λ . This yields a modified particle probability measure

$$\frac{1}{|V_{d,N}|} \cdot \exp(-\beta \cdot U(r)) \cdot \lambda(dr).$$

One immediately notices the similarity to our approach, where we have also used an exponential density $r \mapsto \exp(-\beta \cdot U(r))$. Hereby we have introduced U as being a sum of pair potential functions, from which we have been able to deduce

$$\exp(-\beta \cdot U(r)) = \exp\left(-\beta \cdot \frac{1}{2} \cdot \sum_{i,j \in [N] \neq} u(r_i - r_j)\right) = \prod_{i,j \in [N] \neq} \exp(-\beta \cdot u(r_i - r_j)/2).$$

The difference to Martin-Mayor's now is twofold, as we did not consider an extra normalization factor of $1/|V_{d,N}|$ in our density and our summation includes more particle connections than the *superposition approximation* done in [5]. It only considers direct neighbors in a chained fashion, such that the summation would be

$$\exp(-\beta \cdot U(r)) \stackrel{[5]}{=} \frac{1}{|V_{d,N}|} \cdot \exp\left(-\beta \cdot \sum_{i \in [N-1]} u(r_i - r_{i+1})\right) = \frac{1}{|V_{d,N}|} \cdot \prod_{i \in [N-1]} \exp(-\beta \cdot u(r_i - r_{i+1})).$$

Despite the neglect of further correlations, Martin-Mayor's approach was tested in the context of supercooled liquids in the calculation of coupling coefficients and mode coupling theory. The results were found to be reasonably accurate [5].

Furthermore the paper suggests that the density in superposition approximation can be included into the spring function itself, by defining $f(r) := \exp(-\beta \cdot u(r)) \cdot f(r) / |V_{d,N}|$ for $f(r)$ being the spring function. It is claimed that in the lowest order this would lead to the bare propagator having the form

$$G_0^{(MM)}(\mathbf{p}, z) = \left(z - \rho_* \cdot (\hat{f}(0) - \hat{f}(\mathbf{p})) \right)^{-1}.$$

In our approach this is not the case, as the zeroth order perturbation theory is not affected by the introduced structure factor and therefore remains unchanged.

↪ NUMERICAL ANALYSIS ←

Chapter 4

As a first implementation of the corrected ERM theory we will now discuss a simple repulsive spring function given by

$$\mathbb{R} \ni r \mapsto f_a^{(num)}(r) = \begin{cases} 1 & \text{for } r < a, \\ 0 & \text{else.} \end{cases} \implies \begin{array}{c} f_a^{(num)}(r) \\ \uparrow \\ \text{---} \\ \downarrow \\ r \end{array}$$

This spring function is defined within a finite interaction distance $a \in \mathbb{R}_{>0}$ and is zero elsewhere. The physical application is the model of soft spheres, where overlapping spheres are repelled by a spring force. This model is used in the context of molecular dynamics simulations. [12] To derive the potential given by this interaction we use a technique already applied during the analytical derivation of the pair interaction function in D.2.17, where $[N]^2 \ni (i,j) \mapsto d_{i,j} : R \mapsto R_i - R_j$ came into play. Following the same approach we find for positions $R \in V_{d,N}$ the interaction potential

$$U_a^{(num)}(R) = \sum_{(i,j) \in [N]^2} \underbrace{\begin{cases} \frac{1}{2} \cdot (\|d_{i,j}(R)\|_2 - a)^2 & \text{for } d_{i,j}(R) < a, \\ 0 & \text{else.} \end{cases}}_{=: u_a(d_{i,j}(R))} \implies \begin{array}{c} U_a^{(num)}(d_{i,j}(R)) \\ \uparrow \\ \text{---} \\ \downarrow \\ \|d_{i,j}(R)\|_2 \end{array}$$

Notice that for $a = 1$ we find the same form as [18]. To describe forces induced by the spring potential in d dimensions in our system, we introduce radial symmetry by composing $f_a^{(num)} \circ \|\cdot\|_2$ on any distance $d_{ij}(R)$ of two particles i, j , i.e. we encode the isotropic character of the system into $f_a^{(num)}$. With this we are now ready to calculate the particle probability density $R \mapsto \exp(-\beta \cdot U_a^{(num)}(R))$ in the following.

4.1 Analytical Methods

The idea now is to reduce complexity of the model by using a mean field approach on the particle interaction potential $U_a^{(num)}$. This is done by untangling to direct and indirect contributions towards one specific particle x in R by separation:¹³

$$U_a^{(num)}(x, R_2, \dots, R_N) = 2 \cdot \sum_{j \in [2, N]} u_a(x - R_j) + \sum_{(i,j) \in [2, N]^2} u_a(R_i - R_j),$$

¹³By $[2, N]$ we mean the set $\{2, \dots, N\}$.

and for two particles $x, y \in \mathbb{R}^d$ via

$$U_a^{(num)}(x, y, R_3, \dots, R_N) = 2 \cdot \left(\sum_{j \in [3, N]} u_a(x - R_j) + u_a(y - R_j) + u_a(x - y) \right) + \sum_{(i,j) \in [3, N]^2} u_a(R_i - R_j)$$

where the factor 2 is a result of symmetry $u_a(x - y) = u_a(y - x)$ coming from the norm. The pair distribution function $g_N^{(2)}$ would then be given by

$$g_N^{(2)}(x, R_2) \propto \int_{V_{d,N-2}} \prod_{j \in [N-2]} \exp(-\beta \cdot 2 \cdot (u_a(x - R_j) + u_a(R_2 - R_j) + u_a(x - R_2))) \\ \cdot \prod_{(i,j) \in [N-2]^2} \exp(-\beta \cdot u_a(R_i - R_j)) (\lambda^d)^{N-2}(dR).$$

The radial distribution function $g_{||}(x, \|R_2\|_2)$ then can be calculated by integrating a radial sphere $B_{\|R_2\|_2}(x)$ around the position x , which can be regarded as 0 for large volumes.¹⁴ From this we get

$$\mathbb{R}^d \ni R_2 \mapsto g_0(R_2) = \int_{B_{\|R_2\|_2}(0)} g_N^{(2)}(0, r) \lambda^d(dr).$$

4.1.1 Hypernetted Chain Approximation Method

In general, for low densities $\rho_* \rightarrow 0$ the radial correlation function in a uniform fluid can be written explicitly using the Boltzmann density $\mathbb{R}^d \ni \mathbf{r} \mapsto \exp(-\beta \cdot w(\mathbf{r}))$ [14, eq. 2.6.10] for a pair potential $\mathbb{R}^d \ni R_i - R_j \mapsto w(R_i - R_j)$. Hereby w is called the *potential of mean force*. Uniformity further suggests w to be radially symmetric. This can be founded on a diagrammatical reasoning on the iterative solution of the Ornstein-Zernike equation (introduced shortly in D.4.31). The diagrams arise from the growing composition of integrals (see again 4.31) lead ultimately to a series expansion of the radial distribution function g_{tot} in terms of the density ρ_* of the fluid [16]. This expansion is given by

$$g_{tot}(\mathbf{r}) = \exp(-\beta \cdot w(\mathbf{r})) \cdot \left(1 + \sum_{n=1}^{\infty} \rho_*^n \cdot \tilde{g}_n(\mathbf{r}) \right),$$

where \tilde{g}_n are coefficient functions of g_{tot} 's expansion. From this we can immediately see our claim. Going forward, for higher order terms resulting from higher densities ρ_* one needs to approximate the second factor. This is done by different approaches, known as *closures*. We will take a look at the *hypernetted chain approximation* (HNC) in the following.

Since we in general do not know the mapping of w we use an indirect approach. For this we make use of our radial potential $\mathbb{R}^d \ni \mathbf{r} \mapsto u_a(\mathbf{r})$ by defining the *direct* radial distribution function as $\mathbb{R}_{>0} \times \mathbb{R}^d \ni (a, \mathbf{r}) \mapsto g_{dir}(a, \mathbf{r}) := \exp(-\beta \cdot u_a(\mathbf{r}))$.¹⁵ It makes the contribution of a direct interaction of our reference particle at position $\mathbf{r}_{ref} = 0$ with a particle in $\partial B_r(0) \subset \mathbb{R}^d$, i.e. an other particle at distance $r \in \mathbb{R}$, explicitly. Since there are more than two particles total to be assumed in the system, we provide the *indirect* contribution to the radial distribution

¹⁴Note that the accuracy of the approximation is depending on whether $0 \in V_{d,N-2}$ and on the norm $\|\mathbf{x}\|_2$.

¹⁵By \approx we mean that an approximation in the HNC was done here.

function as

$$g_{ind}(a, \mathbf{r}) := \exp(-\beta \cdot (w(\mathbf{r}) - u_a(\mathbf{r}))),$$

where we virtually subtract the already described direct part u_a from the total potential w . This brings us to $g_{tot}(a, \mathbf{r}) = g_{ind}(a, \mathbf{r}) + g_{dir}(a, \mathbf{r})$, which can be rearranged to

$$g_{dir}(a, \mathbf{r}) = \underbrace{\exp(-\beta \cdot w(\mathbf{r}))}_{\text{total contribution } g_{tot}(\mathbf{r})} - \underbrace{\exp(-\beta \cdot (w(\mathbf{r}) - u_a(\mathbf{r})))}_{\text{indirect contribution } g_{ind}(\mathbf{r})}.$$

Writing the series expansion of the exponential function we further find

$$g_{dir}(a, \mathbf{r}) = \exp(-\beta \cdot w(\mathbf{r})) - \left(1 - \beta \cdot (w(\mathbf{r}) - u_a(\mathbf{r})) + R_2(g_{ind}, 0, \mathbf{r})\right).$$

Assuming that the contribution of the Taylor remainder $R_2(g_{ind}, 0, \mathbf{r})$ is negligible and the difference $w(\mathbf{r}) - u_a(\mathbf{r})$ is small¹⁶, we can further simplify the expression to

$$g_{dir}(a, \mathbf{r}) = \underbrace{g_{tot}(a, \mathbf{r}) - 1}_{=: h(g_{tot}, a, \mathbf{r})} + \beta \cdot (w(\mathbf{r}) - u_a(\mathbf{r})) \approx: c(g_{tot}, a, \mathbf{r}).$$

The newly defined function¹⁷ c is known in literature as the *direct correlation function*, while h is called the *pair correlation function* [16]. Since the total potential w is still unknown, we can express it using already occurring terms by its definition $w(\mathbf{r}) = -\ln(g_{tot}(a, \mathbf{r}))/\beta$ to obtain a fixed point equation for g_{tot} using the *Ornstein-Zernike equation*.

Definition 4.31. Ornstein-Zernike equation.

For $g : \mathbb{R}^d \rightarrow \mathbb{R}$ at a fixed $\mathbf{r} \in \mathbb{R}^d$ the Ornstein-Zernike equation on homogeneous densities $\mathbb{R}^d \ni r' \mapsto \rho(r') = \rho_*$ is given by

$$h(g, r) = h(g, r) + \rho_* \cdot \int_{\mathbb{R}^d} c_a(g, r') \cdot h(g, r - r') \lambda(dr') =: \Phi_{a, \rho_*, r}(g)$$

Thereby $h := g - 1$ and $c(g, a, \mathbf{r}) = g(\mathbf{r}) - 1 + \beta \cdot (w(\mathbf{r}) - u_a(\mathbf{r}))$. If $\Phi_{a, \rho_*, r}$ is a contraction mapping, then g is a solution of the Ornstein-Zernike equation.

The Ornstein-Zernike equation can now be used with the definition of c to find the following hypernetted chain fixed point equation

$$\Phi_{a, r} : g_{tot} \mapsto \underbrace{c(g_{tot}, a, r)}_{\text{direct}} + \underbrace{\int_{\mathbb{R}} c(g_{tot}, a, r') \cdot (g_{tot}(a, r - r') - 1) \lambda(dr')}_{\text{indirect}}, \quad (\text{HCA})$$

which is solved by g_{tot} as a zero of $g \mapsto \Phi_{a, r}(g) - g$, thus approaching the unknown potential function w indirectly. Since we can again see a split of contributions to the indirect and direct

¹⁶Again, where there would be a need of an error estimate, we do not make statements about the quality of the approximation in this work. Please take a look at [19].

¹⁷Notice that in the definitions of c and h (as we have done in g_{tot} , g_{dir} and g_{ind}) we assume β to be constant, otherwise we would write c_β and h_β .

part, the interpretation of the Ornstein Zernike equation becomes clear in the context of our earlier considerations.

4.1.2 Static Structure Factor

If we successively find the fixed point g_{tot} of equation (HCA) we can calculate the static structure factor S_* from lemma 4 by

$$\mathbb{R}^d \ni \mathbf{q} \mapsto S_*(\mathbf{q}) = 1 + \rho_* \cdot \int_{\mathbb{R}^d} \exp(i \cdot \langle \mathbf{q}, \mathbf{r} \rangle) \cdot (g_{tot}(a, \mathbf{r}) - 1) \lambda(d\mathbf{r}). \quad (\text{SSF})$$

For simplicity we stick to a three dimensional space going forward. Since w is radially symmetric, $\mathbb{R}^d \in \mathbf{r} \mapsto g_{tot}(a, \mathbf{r})$ also is a function changing with the vectors norm, i.e. in three dimensions radially symmetric. It turns out to be convenient to make a spherical coordinate transformation and considering $\mathbb{R} \ni r \mapsto g_{|tot|}(a, r)$ going forward.¹⁸ For this we use the cos relation $\cos(\vartheta) \cdot \|\mathbf{q}\|_2 \cdot \|\mathbf{r}\|_2 = \langle \mathbf{q}, \mathbf{r} \rangle$ based on the *Cauchy-Schwarz Inequality* $|\langle \cdot, \cdot \rangle| \leq \|\cdot\| \cdot \|\cdot\|$ for the scalar product of $\mathbf{q}, \mathbf{r} \in \mathbb{R}^3$ to transform the integral:

$$S_*(\mathbf{q}) = 1 + \rho_* \cdot \int_{\mathbb{R}^3} (g_{|tot|}(a, \|\mathbf{r}\|_2) - 1) \cdot \exp(i \cdot \|\mathbf{q}\|_2 \cdot \|\mathbf{r}\|_2 \cdot \cos(\vartheta)) \lambda(d\mathbf{r}).$$

The spherical transformation function $(\rho, \vartheta, \varphi) \mapsto \rho \cdot (\sin(\vartheta) \cdot \cos(\varphi), \sin(\vartheta) \cdot \sin(\varphi), \cos(\vartheta))$ yields a Jacobian determinant of $(\rho, \vartheta) \mapsto \rho^2 \cdot \sin(\vartheta)$, which represents our integral in spherical coordinates as

$$\int_{(-\pi, \pi)} \int_{\mathbb{R}_{>0}} \int_{[0, \pi]} [(g_{|tot|}(a, \rho) - 1) \cdot \exp(i \cdot \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta))] \cdot \rho^2 \cdot \sin(\vartheta) \lambda^3(d\vartheta, d\rho, d\varphi).$$

Evaluation of the outer integral to 2π can be done effortlessly since there appears no dependency on φ . The factor $(g_0(\rho) - 1)$ can be linearly interchanged with $\int_{[0, \pi]}$ such that the inner integral is performed on

$$\mathbb{R} \ni \vartheta \mapsto \sin(\vartheta) \cdot \exp(i \cdot \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta)).$$

Noticing the cos function in the exponential we can use the chain rule of differentiation to find

$$\sin(\vartheta) \cdot \exp(i \cdot \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta)) = -(\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2)^{-1} \cdot \frac{d}{d\vartheta} \exp(i \cdot \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta))$$

for given $\rho \in \mathbb{R}_{>0}$ and $\mathbf{q} \in \mathbb{R}^3$. The differentiation means vanishing integration with respect to ϑ , such that evaluation yields

$$\mathbb{R} \times \mathbb{R}^3 \ni (\rho, \mathbf{q}) \mapsto \frac{\overset{\circ}{i}}{\|\mathbf{q}\|_2 \cdot \rho} \cdot (\exp(-\overset{\circ}{i} \cdot \|\mathbf{q}\|_2 \cdot \rho) - \exp(\overset{\circ}{i} \cdot \|\mathbf{q}\|_2 \cdot \rho)).$$

This basically is the definition of sinc, since $\sin(x) = (e^{\overset{\circ}{i}x} - e^{-\overset{\circ}{i}x})/(2 \cdot \overset{\circ}{i})$ and $\text{sinc}(x) = \sin(x)/x$, such that the mapping is equivalent to $(\rho, q) \mapsto 2 \cdot \text{sinc}(\|\mathbf{q}\|_2 \cdot \rho)$. As a result the integration over \mathbb{R}^3 turns out to be an integration over $\mathbb{R}_{>0}$ with respect to ρ at given wave vectors $\mathbf{q} \in \mathbb{R}^3$ of

¹⁸To recover dimensionality dependencies we write $w_{||}$ defined by $w(\mathbf{r}) = (w_{||} \circ \|\cdot\|_2)(\mathbf{r})$ for $\mathbf{r} \in \mathbb{R}^d$ and $r \mapsto g_{|tot|}(r) := \exp(-\beta \cdot w_{||}(r))$, thus $g_{tot}(\mathbf{r}) = g_{|tot|}(\|\mathbf{r}\|_2)$. The physicist will know that this is meant by radial symmetry of $g_{tot}(\mathbf{r})$.

the Integrand of the static Structure factor relation in Spherical coordinates¹⁹

$$\rho \mapsto 4\pi \cdot (g_{tot}(a, \rho) - 1) \cdot \rho^2 \cdot \text{sinc}(\|\mathbf{q}\|_2 \cdot \rho) \quad (\text{ISS})$$

Notice that the vector arguments \mathbf{q} in no form utilize their directional components, such that the integrand is a radial symmetric function of $\mathbb{R}_{\neq 0} \ni q \mapsto S_{|*|}(q)$. Coming back to equation (SSF) we can now evaluate the integral over $\mathbb{R}_{>0}$ to define a radially symmetric static structure factor $\mathbb{R}_{\neq 0} \ni q \mapsto S_*(q)$ as

$$S_*(\mathbf{q}) = 1 + 4\pi \cdot \rho_* \cdot \int_{\mathbb{R}_{>0}} (g_{|tot|}(a, \rho) - 1) \cdot \rho^2 \cdot \text{sinc}(\|\mathbf{q}\|_2 \cdot \rho) \lambda(d\rho).$$

4.1.3 Dyson Equation Fixed Point Form

The last step now to be taken is to find the fixed point of the Dyson equation in first loop order.

Lemma 6 (Fourier Transform of Heaviside-Based Spring Function). Let $H_a : \mathbb{R} \rightarrow \mathbb{R}$ for $a \in \mathbb{R}_{>0}$ be the Heaviside function defined as

$$H_a(x) := \begin{cases} 1 & \text{if } x < a, \\ 0 & \text{else.} \end{cases} = \mathbb{1}_{[0,a)}(x).$$

Then for 3 dimensional arguments $\mathbf{r} \in \mathbb{R}^3$ the Fourier transform of $F_a(\mathbf{r}) := H_a(\|\mathbf{r}\|_2)$ is given by

$$\mathbb{R}^3 \ni \mathbf{q} \mapsto \hat{F}_a(\mathbf{q}) = 4\pi \cdot (\sin(a \cdot \|\mathbf{q}\|_2) - a \cdot \|\mathbf{q}\|_2 \cdot \cos(a \cdot \|\mathbf{q}\|_2)) \cdot \|\mathbf{q}\|_2^{-3}.$$

Furthermore it has a removable singularity at $\mathbf{q} = 0$ with $(\mathcal{F}F_a)(\mathbf{0}) = 4\pi a^3/3$. From its radial symmetry the existence of $\hat{F}_{a,\parallel} : \mathbb{R} \rightarrow \mathbb{R}$ with $\hat{F}_a = \hat{F}_{a,\parallel} \circ \|\cdot\|_2$ follows.

The proof is given in the Appendix. With this we can define the bare propagator $\mathbb{R}^3 \times \mathbb{C} \ni (\mathbf{p}, z) \mapsto G_0(\mathbf{p}, z)$ and the Vertex function $(\mathbb{R}^3)^2 \ni (\mathbf{q}, \mathbf{p}) \mapsto V(\mathbf{q}, \mathbf{p})$ both are needed for the self energy $\mathbb{R}^3 \times \mathbb{C} \ni (\mathbf{p}, z) \mapsto \Sigma^{(1)}(\mathbf{p}, z)$. The first function is given by

$$\mathbb{R}^3 \times \mathbb{C} \ni (\mathbf{p}, z) \mapsto G_0(\mathbf{p}, z) = \frac{1}{z - \rho_* \cdot (\hat{F}_a(\mathbf{0}) - \hat{F}_a(\mathbf{p}))},$$

whereas the vertex function is given by

$$\mathbb{R}^2 \ni (\mathbf{q}, \mathbf{p}) \mapsto V(\mathbf{q}, \mathbf{p}) = \rho_* \cdot (\hat{F}_a(\mathbf{q}) - \hat{F}_a(\mathbf{q} - \mathbf{p})).$$

From this we are already able to build up the integral representation which we will use as our fixed point iteration for the propagator $(\mathbf{p}, z) \mapsto G(\mathbf{p}, z)$ in the first loop order. It is firstly of

¹⁹Pun intended.

the form

$$G \mapsto \frac{G_0(\mathbf{p}, z)^2}{\rho_*} \cdot \int_{\mathbb{R}^3} S_*(\mathbf{q}) \cdot G(\mathbf{p} - \mathbf{q}, z) \cdot V(\mathbf{q}, \mathbf{p})^2 \lambda(d\mathbf{q}),$$

where we again need to spherically deal with the three dimensional integral. But before we do so, since our goal is numerical analysis, we will have to discretize the integral later on. Since we need to iterate over discrete evaluations of G at gridpoints \mathbf{q}_i , we transform the integral linearely with $\mathbf{q} \mapsto \mathbf{p} - \mathbf{q}$ to get

$$G \mapsto G_0(\mathbf{p}, z) \cdot \left(1 + \frac{G_0(\mathbf{p}, z)}{\rho_*} \cdot \int_{\mathbb{R}^3} S_*(\mathbf{p} - \mathbf{q}) \cdot G(\mathbf{q}, z) \cdot V(\mathbf{p} - \mathbf{q}, \mathbf{p})^2 \lambda(d\mathbf{q}) \right)^{-1}.$$

Conveniently we have proven a symmetry in V during its introduction in TD.2.2, which unveils a simplification $(V(\mathbf{p} - \mathbf{q}, \mathbf{p}))^2 = (-1)^2 \cdot (-V(\mathbf{p} - \mathbf{q}, \mathbf{p}))^2 = V(\mathbf{q}, \mathbf{p})^2$. Lastly using D.2.28 and the geometric series by preasssuming $\int_{\mathbb{R}^3} S_*(\mathbf{p} - \mathbf{q}) \cdot G(\mathbf{q}, z) \cdot V(\mathbf{q}, \mathbf{p})^2 \lambda(d\mathbf{q}) \cdot G_0(\mathbf{p}, z)^2 / \rho_* \in [0, 1)$ the fixed point form convertes to

$$G \mapsto \left(G_0(\mathbf{p}, z)^{-1} - \rho_*^{-1} \cdot \int_{\mathbb{R}^3} S_*(\mathbf{p} - \mathbf{q}) \cdot G(\mathbf{q}, z) \cdot V(\mathbf{q}, \mathbf{p})^2 \lambda(d\mathbf{q}) \right)^{-1}.$$

Later on we can use a matrix representation for the integral of the form $\text{IntM} \cdot G_v$ due to the grid $Q = \{q_1, \dots, q_{n_q}\}$. But before doing so we continue the analytic discussion. Performing the spherical transformation by again using $\Phi : (\rho, \vartheta, \varphi) \mapsto \rho \cdot (\sin(\vartheta) \cdot \cos(\varphi), \sin(\vartheta) \cdot \sin(\varphi), \cos(\vartheta))$ we get

$$\int_{(-\pi, \pi)} \int_{\mathbb{R}_{>0}} \int_{[0, \pi]} \left[S_*(\mathbf{p} - \Phi(\vartheta, \rho, \varphi)) \cdot G_{||}(\rho, z) \cdot V(\Phi(\vartheta, \rho, \varphi), \mathbf{p})^2 \right] \cdot \rho^2 \cdot \sin(\vartheta) \lambda^3(d(\vartheta, \rho, \varphi)).$$

It was easy to replace \mathbf{q} with ρ within $G_{||}$ since we directly have $G_0 = G_{|0|} \circ ||\cdot||_2$ from $\hat{F}_a = \hat{F}_{a,||} \circ ||\cdot||_2$ for scalar Functions $G_{|0|}$ and $F_{a,||}$, see L.6. Following the iteration of the fixed point equation, this radial symmetry is reserved for all following propagators.

For the other functions we have to be more careful. With $\mathbf{p} \in \mathbb{R}^3$ we have

$$\|\mathbf{p} - \Phi(\vartheta, \rho, \varphi)\|_2^2 = \|\mathbf{p}\|_2^2 + \rho^2 - 2 \cdot \langle \mathbf{p}, \Phi(\vartheta, \rho, \varphi) \rangle,$$

where $\|\Phi(\vartheta, \rho, \varphi)\|_2 = \rho$. From the radial symmetry in \mathbf{p} we can freely choose the particular direction of \mathbf{p} . Looking at the spherical transformation Φ we decide on $\mathbf{p} = \|\mathbf{p}\|_2 \cdot e_3$ such that

$$\langle \mathbf{p}, \Phi(\vartheta, \rho, \varphi) \rangle = \|\mathbf{p}\|_2 \cdot \cos(\vartheta) \cdot \rho.$$

Furthermore the norm is now accessible by only ρ , ϑ and $\|\mathbf{p}\|_2$, such that a scalar function can be used:

$$\|\mathbf{p} - \Phi(\vartheta, \rho, \varphi)\|_2^2 \stackrel{\mathbf{p}=p \cdot e_3}{=} p^2 + \rho^2 - 2 \cdot p \cdot \rho \cdot \cos(\vartheta) =: N(p, \rho, \vartheta).$$

Defining $\mathbb{R}^2 \ni (x, y) \mapsto V_{||}(x, x - y) := \rho_* \cdot (\hat{F}_{a,||}(x) - \hat{F}_{a,||}(x - y))$ we hereby get the integrand

$$(p, \vartheta, \rho) \mapsto S_{|*|}(N(p, \rho, \vartheta)) \cdot G_{||}(\rho, z) \cdot V_{||}(\rho, N(p, \rho, \vartheta))^2 \cdot \rho^2 \cdot \sin(\vartheta). \quad (27)$$

Since we can already see the independence of φ due to the direction of \mathbf{p} the integral $\int_{(-\pi, \pi)} \dots \lambda(d\varphi)$ is easily evaluated to 2π . Setting $\text{Int}(\mathbf{p}, \vartheta, \rho) := 2\pi \cdot (27)$ we can now formulate the fixed point equation based on the dyson formalism that is used in the following numerical analysis for arguments $(p, z) \in \mathbb{R} \times \mathbb{C}$ as

$$G \mapsto \left(z - \rho_* \cdot (\hat{F}_{a,||}(0) - \hat{F}_{a,||}(p)) - (\rho_*)^{-1} \cdot \int_{\mathbb{R}_{>0}} \int_{[0, \pi]} \text{Int}(\mathbf{p}, \vartheta, \rho) \lambda^2(d(\vartheta, \rho)) \right)^{-1}. \quad (\text{DF})$$

Now the question of implementation remains to be discussed.

4.2 Numerical Methods

For the implementation we decide to use the programming language Julia for its high performance, flexibility and the ability to write code that is close to mathematical notation. Our implementation therefore requires the following packages:

```

1 using Distributed
2 using OrnsteinZernike, GLMakie, FFTW, Statistics, ProgressMeter,
   QuadGK, NLSolve, ForwardDiff, LinearAlgebra, LoopVectorization,
   Base.Threads, CSV, DataFrames

```

To get the basics out of the way, for $d = 3$ and $kBT = 1$ we define on the parameter tuple $p = (1.0, 2.0, 1.0)$ the spring function f and the potential U_{neu} as

```

1 @everywhere function HeavisideSpring(r, p)
2   if r < p[3]
3     return 1
4   else
5     return 0
6   end
7 end
8
9 @everywhere function U_HeavisideSpring(r, p)
10  if r < p[3]
11    return 0.5 * (r - p[1])^p[2]
12  else
13    return 0
14  end
15 end

```

The `@everywhere` macro is used in Julia for distributed computing.

Numerical HNC Approximation

The implementation of the hypernetted chain fixed point equation from (HCA) turns out to be tricky, since our fixpoint essentially needs to be a function of $r \in \mathbb{R}$. It is also needed to evaluate

a folding with $r' \mapsto g_{tot}(r - r') - 1$. For a fixed $a \in \mathbb{R}$ the implementation can be done via

```

1 g_hca = r -> exp(-β * U_num(r))
2 c_hca = (g, r) -> g(r) - 1 - log(g(r)) - β * U_num(r)
3 int_hca = (g, r) -> hcubature(
4     rs -> c_hca(g, rs) * (g_hca(r - rs) - 1),
5     [vol_min for dim in 1:length(r)],
6     [vol_max for dim in 1:length(r)],
7     rtol=1e-5
8 )[1]
9 Φ_hca = g -> r -> c_hca(g, r) + int_hca(g, r)

```

and a following iteration over g , which in our testing turned out to converge very slowly. Instead we will use the work of Ilian Pihlajamaa on his GitHub repository [IlianPihlajamaa/OrnsteinZernike.jl](#) for a more efficient implementation and straightforward implementation.²⁰

```

1 # -> Define system potential (model)
2 potential = CustomPotential(Uf, params)
3
4 # -> Create System struct
5 system = SimpleLiquid(d, ρ, kBt, potential)
6
7 # -> Define solving closure
8 closure = HypernettedChain()
9
10 # -> generate solution from system parameters
11 solution = @time solve(system, closure)

```

This yields a solution object with `solution.r` as the radii that g has been evaluated on and `solution.gr` as the corresponding values of g . For the first we also use the Symbol G_r to denote the grid points of r .

Numerical Structure Factor

Now we are ready to discretize the integral $\int_{\mathbb{R}_{>0}}$ on $[0, R]$ for $R > 0$ given by $R = \max(G_r)$ with respect to ρ as

$$\int_{[0,R]} (\text{ISS}) d\rho \approx \sum_{\rho \in G_r} 4\pi \cdot (g(\rho) - 1) \cdot \rho^2 \cdot \text{sinc}(\rho \cdot q) \cdot \Delta\rho.$$

By default we work with a grid resolution of 1024 points. To test and enhance convergence this is altered but not explicitly mentioned in the following. The discretized integral can now be implemented via

²⁰Again, I want to express my gratitude to Ilian Pihlajamaa for his amazing work on this package.

```

1 cFT_integrand = (q,r) -> 2 * sinc(q * r)
2 cFT = q -> begin
3     if exp_g_toggle
4         sum(r^2 * 2 * pi * (exp(-1 * Uf(r, params)) - 1) * x
5             * Δr for (x,r) in zip(cFT_integrand.(q, solution
6             .r), solution.r))
7     else
8         sum([r^2 * 2 * pi * gm * x * Δr for (x, gm, r) in zip(
9             cFT_integrand.(q, solution.r), [x - 1 for x in
10            solution.gr], solution.r)]) # use cFT_integrand on
11            all r values from solution.r, then discretely
12            integr.
13    end
14 end

```

Hereby `exp_g_toggle` is a boolean that switches between the Heaviside and the exponential spring function later on. To finally calculate the static structure factor, which now also has radial symmetry $\mathbb{R} \ni \mathbf{q} \mapsto S_*(\mathbf{q})$, we simply take the real part of $q \mapsto \text{cFT}(q)$ with the following code

```

1 S_k = q -> 1 + ρ * real(cFT(q))

```

Numerical Dyson Fixed Point Equation

For the numerical structure factor we need to calculate the fourier transformed spring function \hat{F}_a from L.6. Plotting in one dimension gives us the graph shown in Figure 7. Notice that \hat{F}_1 has its maximum at $\omega = 0$ and decays to 0 for $\omega \rightarrow \infty$.

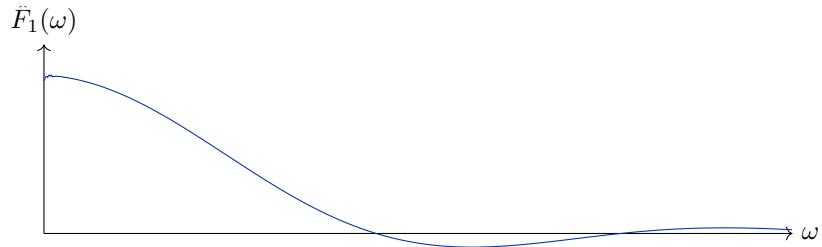


Figure 7: Graphical representation of the Fourier transform \hat{F}_1 of the Heaviside spring function $F_1 := H_a \circ \|\cdot\|_2$ in three dimensions. The argument domain is $\omega \in [0, 10]$.

Since around $\omega = 0$ the function has a removable singularity, for numerical stability it *can* be helpful to use an approximation of \hat{F}_a using its Taylor expansion for small ω as

$$\hat{F}_a(\|\mathbf{q}\|_2) = \frac{4\pi a^3}{3} - \frac{2\pi a^5 \|\mathbf{q}\|_2^2}{15} + \frac{\pi a^7 \|\mathbf{q}\|_2^4}{210} + \mathcal{O}(\|\mathbf{q}\|_2^6).$$

However it does not guarantee better results, as our numerical tests have shown. Nevertheless its implementation in Julia reads

```

1  @everywhere function FHeavisideSpring_1d(ω)
2      local p = params
3
4      if ω == 0.0
5          return 4 * pi * p[3]^3/3
6      # elseif ω < 0.01
7          # return ((4*pi)/(3)) - ((2*ω^2*pi)/(15)) + ((ω^4*pi)/(210))
8          # - ((ω^6*pi)/(11340)) + ((ω^8*pi)/(997920)) - ((ω^10*pi)/(129729600));
9      else
10         return 4 * pi * (sin(p[3] * ω) - p[3] * ω * cos(p[3] * ω)) *
11             ω^(-3)
12     end
13 end
```

The integral found for the Dyson fixed point equation in (DF) now needs to be discretized and implemented. Herefor we choose a grid $Q = \{q_1, \dots, q_{n_q}\}$ with $q_1 = \varepsilon$ and $q_{n_q} = q_{\max} - \Delta q$, with equal spacing to begin with. The maximum value q_{\max} is set to 30, but also altered later on due to numerical instabilities in some regions. For the domain of angles we choose $\{\vartheta_1, \dots, \vartheta_{n_\vartheta}\}$ with $\vartheta_1 = 0$ and $\vartheta_{n_\vartheta} = \pi - \Delta\vartheta$ with equal spacing $\Delta\vartheta = \pi/n_\vartheta$. This lets us approximate the integrand as

$$I : p \mapsto S_{|*|} \left(\sqrt{p^2 + q_i^2 - 2 \cdot p \cdot q_j \cdot \cos(\vartheta_k)} \right) \cdot V_{||} \left(\sqrt{q_i, p^2 + q_i^2 - 2 \cdot p \cdot q_i \cdot \cos(\vartheta_i)} \right)^2 \cdot q_i^2 \cdot \sin(\vartheta_i).$$

The integration now includes the widths Δq and $\Delta\vartheta$. All together, we have

$$\int_{\mathbb{R}_{>0}} \int_{[0, \pi)} (\text{DF}) d\vartheta d\rho \approx \sum_{q \in Q} \sum_{\vartheta \in \Theta} I_{q, \vartheta}(p) \cdot \Delta q \cdot \Delta\vartheta.$$

Notice now that $(p, q) \mapsto I_{q, \vartheta}(p)$ on gridpoints Q will yield a matrix of sums over angles, which can be used to represent the integration. Defining $\text{IntM}(i, j) := I_{q_i, \cdot}(q_j)$ we can write the integral as

$$\int_{\mathbb{R}_{>0}} \int_{[0, \pi)} (\text{DF}) d\vartheta d\rho \approx \text{IntM} \cdot G_v,$$

Where $G_v := (G(q_i, z))_{i \in [n_q]}$ is the discrete propagator vector. The implementation of this idea reads:

```

1 BarePropagator = (ω, z) -> 1 / (z - ρ * (Ff(0) - Ff(ω)))
2 Vertex = (x, y) -> (Ff(x) - Ff(y))
3
4 Integrand = Gv -> (p, q, θ) -> begin
```

```

5      norm_val = NormPminusSph_safe(p, q, theta)
6      if norm_val <= 0
7          throw(ArgumentError("Norm value is negative at p = $p, r = $q, theta = $theta"))
8      end
9      if structure_factor_toggle
10         return S_safe(norm_val) * Vertex(q, norm_val)^2 * q^2 * sin(theta)
11             * (2 * pi)^(-2)
12     else
13         return 1 * Vertex(q, norm_val)^2 * q^2 * sin(theta) * (2
14             * pi)^(-2)
15     end
16 end
17
18 # -> Build Integration matrix
19 IntegrationMatrix = zeros(length(Q), length(Q))
20
21 # -> Fill Integration matrix
22 @time @showprogress @threads for i in 1:length(Q)
23     p = Q[i]
24     for j in 1:length(Q)
25         q = Q[j]
26         if j == 1
27             IntegrationMatrix[j, i] = sum(Integrand(Gv)(p
28                 , q, theta) * Delta_theta for theta in thetaRange)
29         else
30             IntegrationMatrix[j, i] = sum(Integrand(Gv)(p
31                 , q, theta) * Delta_theta for theta in thetaRange) * (Q[j] - Q[j
32                 - 1])
33         end
34     end
35 end
36
37 end

```

Hereby the norm function $N(p, \rho, \vartheta)$ is implemented accordingly, while avoiding division by zero:

```

1 NormPminusSph_safe = (p, r, theta) -> begin
2     norm_val = (p^2 + r^2 - 2 * p * r * cos(theta))^0.5
3     if norm_val <= 0
4         norm_val = eps()
5     end
6     return norm_val
7 end

```

The iteration now is done over the propagator definition, where

$$G_v(i) \mapsto \frac{1}{z - \rho \cdot (\hat{F}_1(0) - \hat{F}_1(q)) - \rho^{-1} \cdot (\text{IntM} \cdot G_v)_i}$$

states the value of G at a gridpoint q_i .

```

1 MDiscreteOneLoopSelfEnergy = Gv -> (IntegrationMatrix * Gv)
2
3 # -> Define Iterator function
4 MIerator = Gv -> [(z - ρ * (Ff(0) - Ff(p)) - ρ *
    MDiscreteOneLoopSelfEnergy(Gv)[i])^(-1) for (i, p) in enumerate(Q)
]

```

The iteration is done using the package `NLsolve` in Julia, such that the following code can be used:

```

1 z = 0.0
2 initial_Gv = Gv(0.0)
3
4 result = @time fixedpoint(x -> MIerator(x), initial_Gv, show_trace
    = true, ftol=1e-2, iterations = iterations_count)

```

For small densities ρ_* an other approximation can be done, by changing the radial distribution function from its definition to an exponential ansatz defined by $g_{exp} : \mathbf{r} \mapsto \exp(-u_a(\mathbf{r})) = \exp(-(||\mathbf{r}||_2 - a)^2/2)$, which essentially is stated by our potential $u_a(r)$ that resulted in the chapters introduction from the spring function $f_a^{(num)}$.

Another ansatz is a gaussian spring function $f^{(gau\beta)} : r \mapsto \exp(-r^2/2)$. For its implementation the Fourier transformed spring function in three dimensions is needed. Since the integral at hand yields

$$\begin{aligned} (\mathcal{F}(f^{(gau\beta)} \circ ||\cdot||_2))(\mathbf{q}) &= 2\pi \cdot \int_{\mathbb{R}_{>0}} \int_{[0,\pi]} \exp\left(\frac{-\rho^2}{2}\right) \cdot \rho^2 \cdot \sin(\vartheta) \cdot \exp(i \cdot \rho \cdot ||\mathbf{q}||_2 \cdot \cos(\vartheta)) \lambda(d\vartheta) \lambda(d\rho) \\ &= 4\pi \cdot \int_{\mathbb{R}_{>0}} \exp\left(\frac{-\rho^2}{2}\right) \cdot \rho^2 \cdot \text{sinc}(\rho \cdot ||\mathbf{q}||_2) \lambda(d\rho), \end{aligned} \quad (28)$$

only the generated potential function is left to be evaluated. For it there are two integrations needed:²¹

$$U^{(gau\beta)}(r) = \int_{(0,r)} \int_{(0,\rho)} \exp\left(-\frac{\xi^2}{2}\right) \lambda(d\xi) \lambda(d\rho) = \sqrt{\frac{\pi}{2}} \cdot r \cdot \text{erf}\left(\frac{r}{\sqrt{2}}\right) + \exp\left(-\frac{r^2}{2}\right) - 1.$$

Hereby $\text{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x \exp(-t^2) dt$ is the error function. Although the principal implemen-

²¹The result can be verified by using a symbolic computation software like Wolfram Alpha. One can use the input `Integrate[Integrate[exp(-x^2/2), {x, 0, y}], {y, 0, t}]`. As we do not discuss this model in this thesis, we will not give further proof.

tation is straightforward, we encountered numerical errors while evaluation within our time constraints, such that this model cannot be discussed in this thesis.

4.3 Numerical Results

Using the approximations and techniques discussed in the previous sections we were able to make several observations. To begin with, the *radial distribution function* for our system, which is given by a quadratic pair potential function $r \mapsto 0.5 \cdot (r - 1)^2$ resulting from the chosen spring function, has the predicted course and does converge to 1, as one can see in Figure 8.

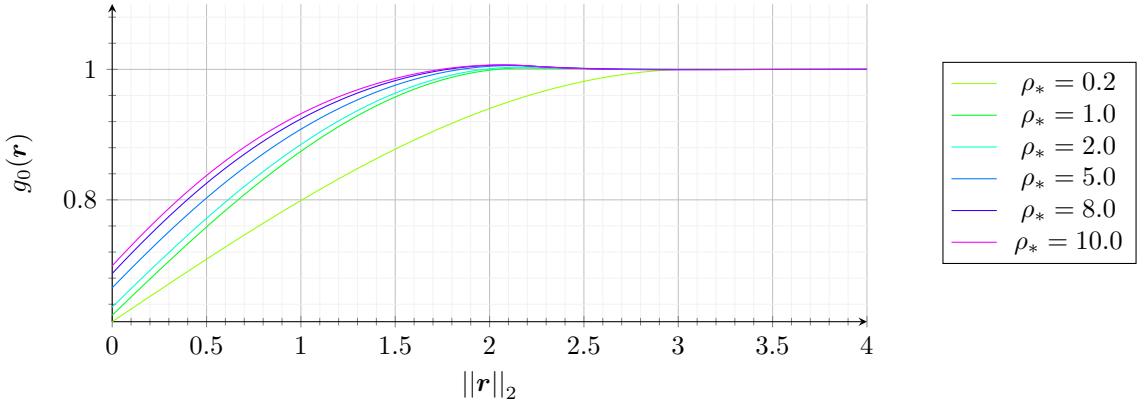


Figure 8: The radial distribution function $\mathbf{r} \mapsto g_0(\mathbf{r}) = g_{|(|0, \|\mathbf{r}\|_2)}^{}(0)$ on a general scale.

It gives, as we have seen in previous chapters, a measure of the probability of finding a particle at a distance $r \in \mathbb{R}_{>0}$ from another particle. Having a maximum at 2 is by construction of the potential and hard-coded into the spring function, since we can interpret the scalar a as a particle diameter. In a general course one also notices, that the starting amplitude near $\|\mathbf{r}\|_2 = 0$ increases with density ρ_* . Since we have a soft sphere model at hand, overlapping of particles is not *forbidden* but rather restricted by the potential function. For growing densities however, it comes natural that particle overlap is more likely. The convergence to 1 furthermore suggests, that for large distances the information about particle probability is lost and therefore finalizes in a uniform distribution.

One can also directly observe a small shift and increase in the maximum of the radial distribution function g_0 as the density ρ_* increases. This can be seen when zooming in on the maximum of the function, as shown in Figure 9. Notice that we do not see a region of g_0 being nearly zero for small radii, as it was the case in our example in figure 5. This clearly is expected, since we use a different potential function here. A similar form to the previous example would be gained by using the Lennard-Jones potential.

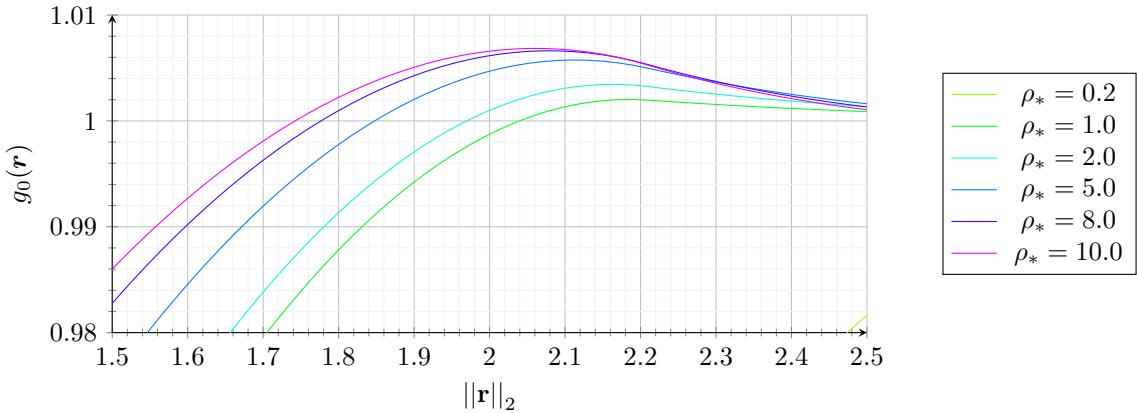


Figure 9: The radial distribution function $\mathbf{r} \mapsto g_0(\mathbf{r}) = g_{||}(0, \|\mathbf{r}\|_2)$ on a small scale around its maximum.

To proceed, the static structure factor S_* can now be drawn in figure 10 using the calculated distribution function from solving the Ornstein-Zernike equation. Noticeable is that the for all tested densitys the value of S_* is constantly bigger than 0.0, which is a good sign for physical applicability. The value of S_* can be related to compressibility using the *compressibility relation*

$$S_*(0) = 1 + \rho_* \cdot \int_{\mathbb{R}^3} (g_0(\mathbf{r}) - 1) \cdot \exp(i \cdot \mathbf{r} \cdot 0) \lambda(d\mathbf{r}) = \frac{\langle N^2 \rangle - \langle N \rangle^2}{\langle N \rangle} = \rho_* \cdot k_B \cdot T \cdot \kappa_T,$$

where κ_T is the isothermal compressibility. Since $\langle N^2 \rangle \geq \langle N \rangle$ the compressibility cannot be negative [12].

As it can be seen in figure 10 the structure factor is getting increasingly smaller with larger density values. This can be related to our model: with increasing density in a volume V the particle count needs to increase, which results in a smaller volume that can be occupied by a single particle. This means that on average particle movement is more restricted. In compressibility terms, this means that at isothermal conditions the system reacts less to changes in pressure by changing its volume. Its growth for larger wave vector norms can be explained by the fact that the particles are more likely to be found in a certain distance to each other. This correlates with nuclear shells, where particles also tend to be found in certain distances to each other.

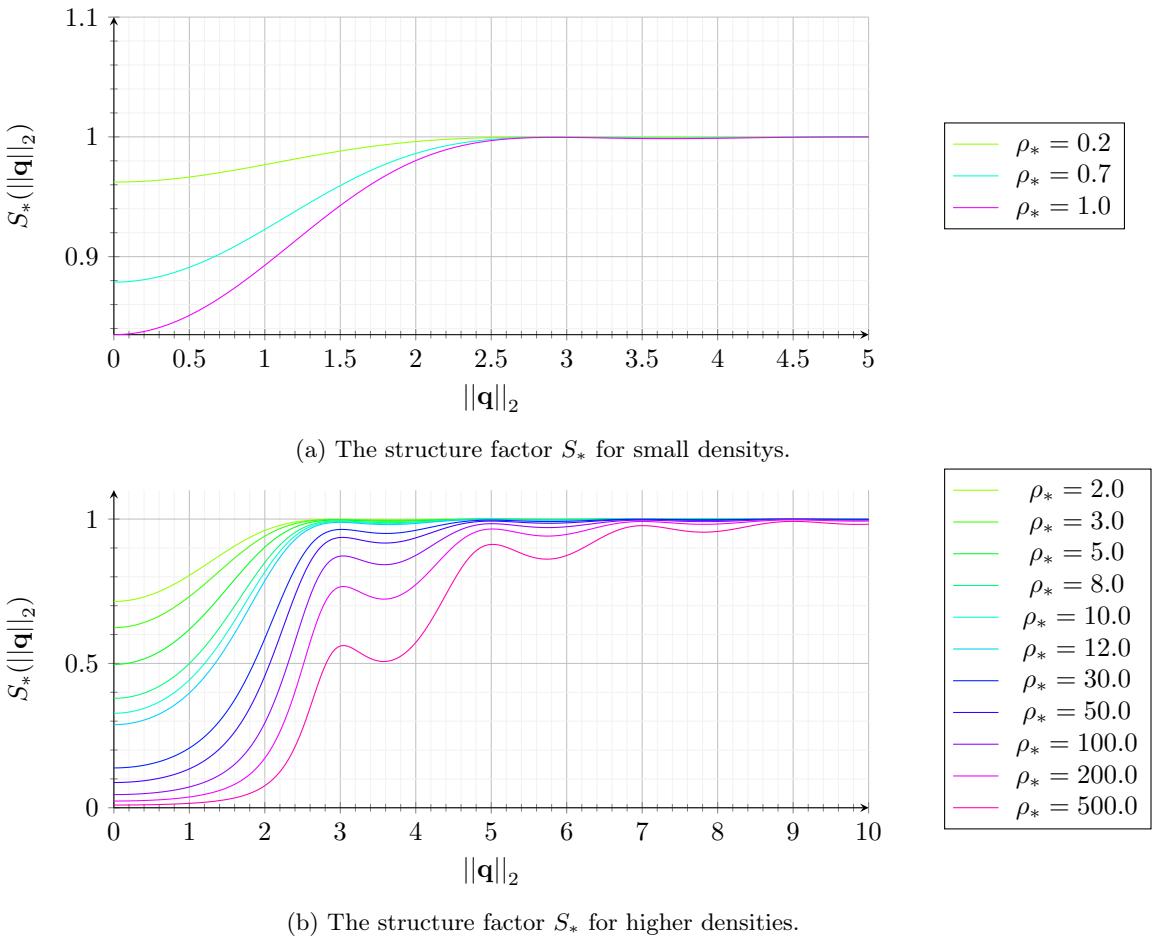
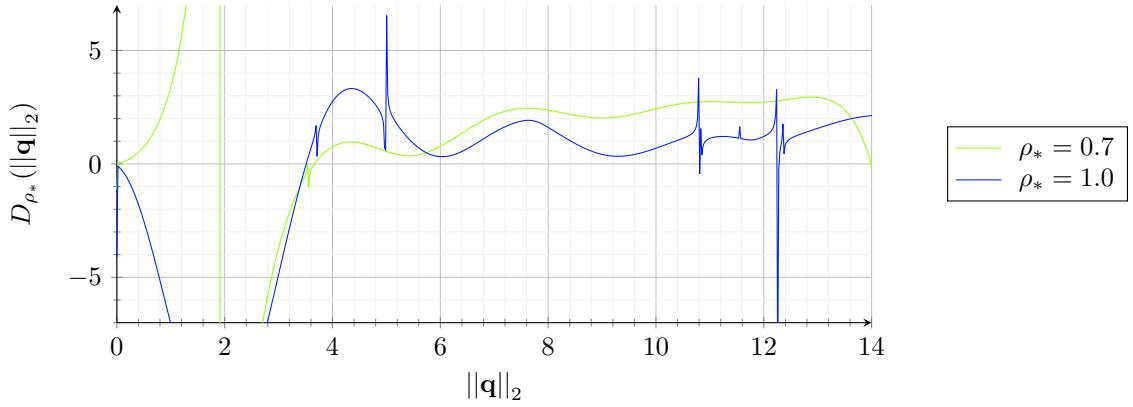
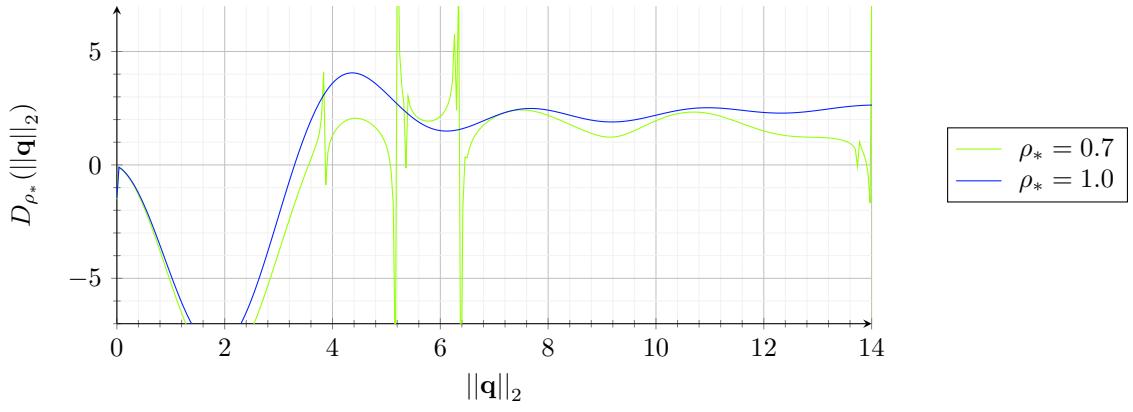


Figure 10: Combined view of the structure factor S_* for small and higher densities ρ_* .

Calculating the corresponding solutions $\rho_* \mapsto G_{fix,\rho_*}$ to the Dyson fixed point equation using as an initial guess the function $G_{0,\rho_*}(q) = (0 - \rho_* \cdot (\hat{F}_a(0) - \hat{F}_a(q)))^{-1}$ for norms $q = \|\mathbf{q}\|_2$, the dispersion relation given by the negative inverse $D_{\rho_*}(q) = -G_{fix,\rho_*}(q)^{-1}$ shows interesting behaviour. As one can see in figure 11, the dispersion relation D_{ρ_*} for small densities ρ_* is not purely positive for wave vector norms between 0.0 and 4.0. But the first inevitable observation is the introduction of numerical instabilities, especially in the calculations for $S_*(q) = 1.0$ for small densities. This creates spikes in figure 11a without any physical meaning and make the data hard to interpret, since a general course is hardly observable.



(a) The structure factor is set to $S_*(q) = 1.0$ for all densitys.



(b) The structure factor is set to $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}g_0 - 1.0)(q)$ for all densitys.

Figure 11: The dispersion relation D_{ρ_*} for small densitys ρ_* .

Nevertheless the dispersion relation $||\mathbf{q}||_2 \mapsto D_{\rho_*}(||\mathbf{q}||_2)$ for small densitys with the corrected static structure factor involved show a more stable behaviour. After the first window of wave vectors q with norm values smaller than 4.0 the dispersion relation becomes purely positive and shows an oscillating behaviour.

Increasing the density ρ_* in a range starting from 2.0 to 12.0 the minimum of the dispersion relation shifts monotonously to the origin, i.e. D_{ρ_*} becomes positive for smaller wave vectors q with increasing densities. Also from a numerical perspective the convergence to a fixed point is achieved in a much more stable manner. This can be seen in figure 14. Again a smoothing character of the static structure factor S_* can be observed.

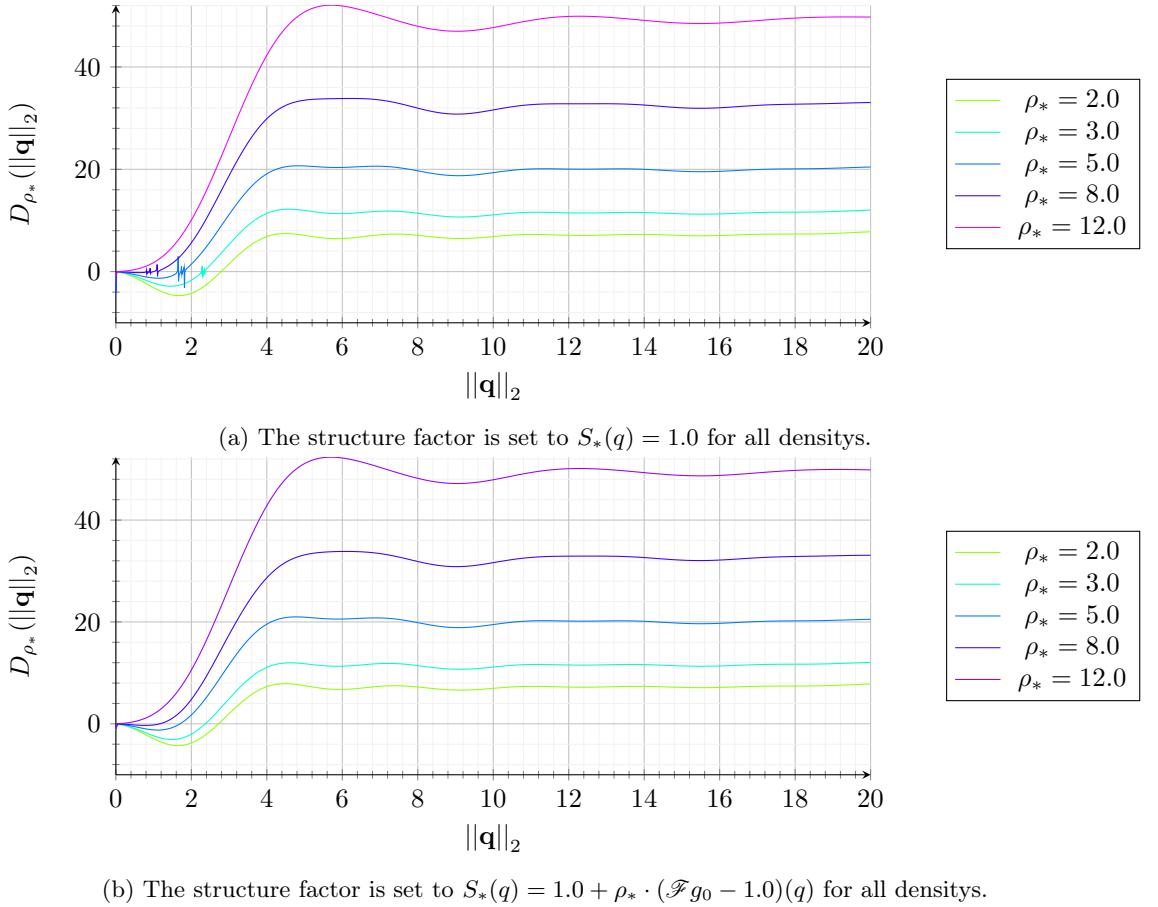


Figure 12: The dispersion relation $D_{\rho_*}(\|q\|_2)$ with S_* for higher densities.

In direct comparison with the dispersion relation with a constant structure factor $S_*(q) = 1.0$ it is apparent that the values are almost identical. Taking a closer look however shows that there is an ever so slight increase in the amplitude.

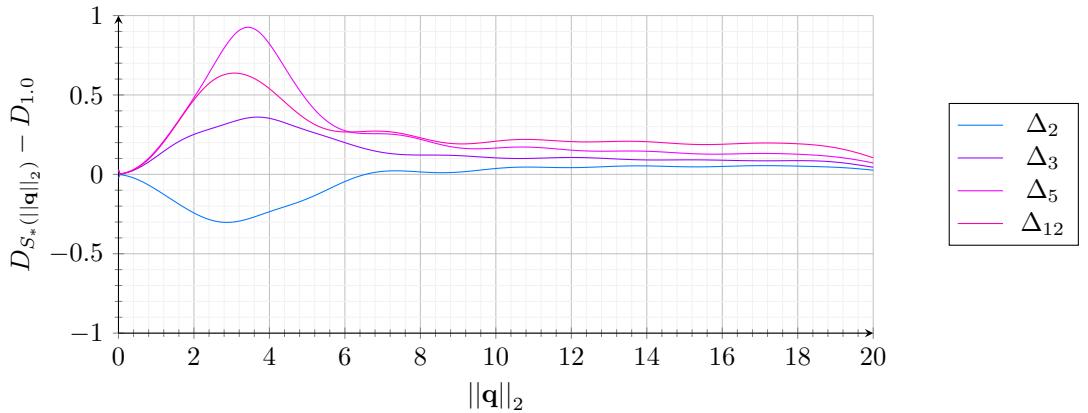


Figure 13: Comparison of the dispersion relation D_{ρ_*} for $\rho_* = 5.0$ with $S_*(q) = 1.0$ and $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}g_0 - 1.0)(q)$. It is drawn $D_{S_*(q)} - D_{1.0}$ for $D_{S_*(q)}$ the dispersion relation with the corrected structure factor. A positive value means that dispersion with static structure factor yields a higher amplitude.

On a broader scale the optical equality of graphs stays apparent, see in direct comparison in figure 14.

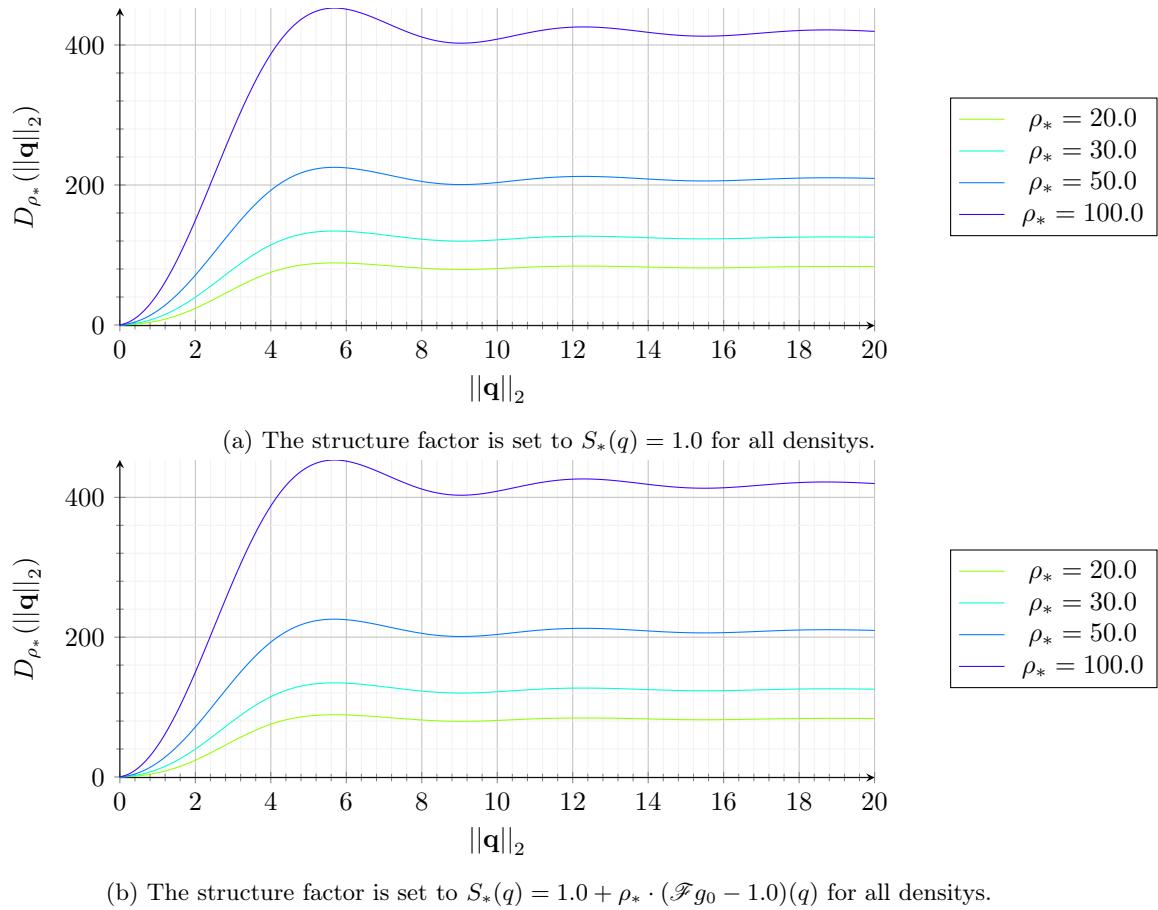


Figure 14: The dispersion relation $D_{\rho_*}(\|\mathbf{q}\|_2)$ with S_* for higher densitys.

Looking at the minimum of the dispersion relation with and without the corrected structure factor gives us an idea when the model becomes more and more physically applicable, see figure 15.

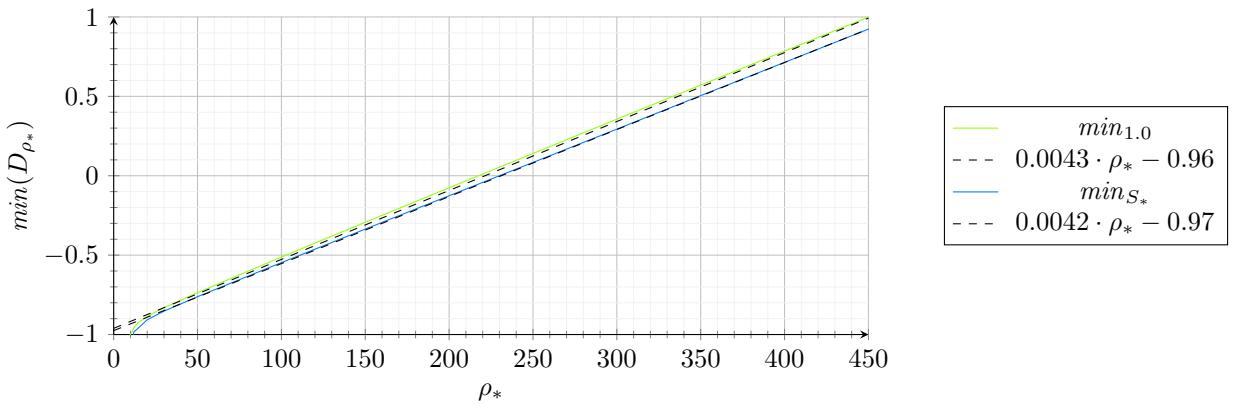


Figure 15: The minimum of the dispersion relation D_{ρ_*} for different densities ρ_* with $S_*(q) = 1 + \rho_* \cdot (\mathcal{F}g_0 - 1.0)(q)$.

It can be seen that scaling with linear fitting is nearly identical for both cases. The critical point where the dispersion relation becomes purely positive can be approximated by linear regression and solving for 0, i.e. $\rho_{*,0} \approx 221.35$.

Another comparison by plotting the difference of the dispersion relations shows a minor increase in the amplitude, that is completely neglectable with regard to the overall behaviour.

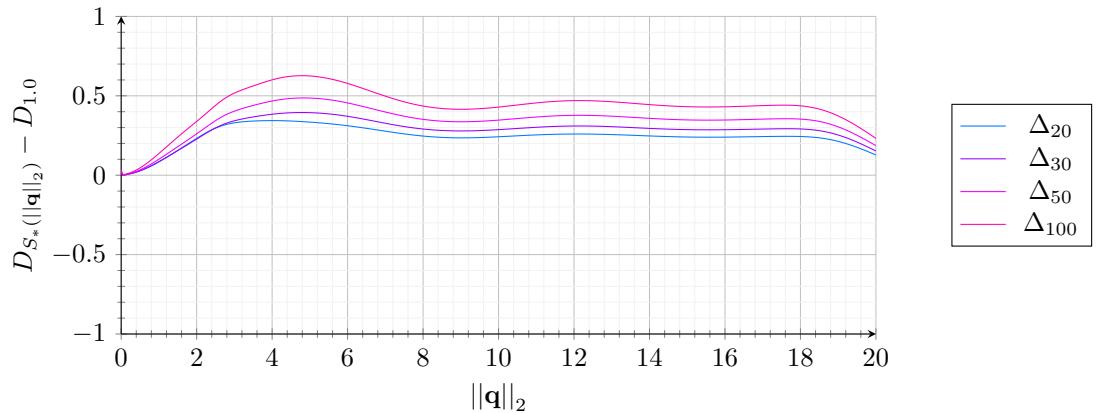


Figure 16: Comparison of the dispersion relation D_{ρ_*} for $\rho_* = 5.0$ with $S_*(q) = 1.0$ and $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}g_0 - 1.0)(q)$. It is drawn $D_{S_*(q)} - D_{1.0}$ for $D_{S_*(q)}$ the dispersion relation with the corrected structure factor. A positive value means that dispersion with static structure factor yields a higher amplitude.

Evaluating the velocity of sound $c_{\rho_*} = \text{mean}_{q \in G_q}(\sqrt{D_{\rho_*}(q)}/q)$ for different densities ρ_* yields the graph shown in figure 17. One can see a small increase of amplitude in a density region of $\rho_* \in [2.0, 12.0]$. Afterward the amplitudes of corrected and uncorrected dispersion relations are effectively identical, as figure 14 shows.

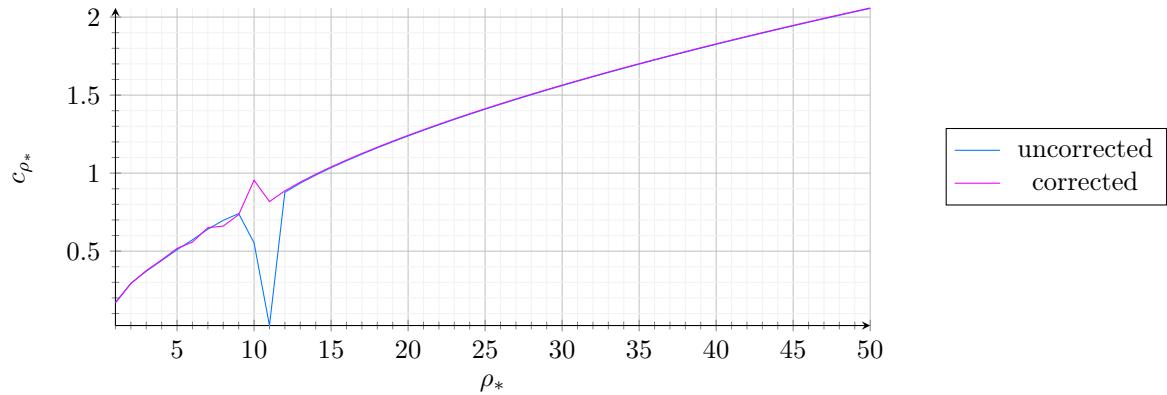


Figure 17: The velocity of sound c_{ρ_*} for different densities ρ_* in comparison with $S_*(q) = 1.0$ and $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}(g_0 - 1))(q)$.

Note that the spike at $\rho_* = 11.0$ is a result of no convergence in the calculation of the dispersion relation.

The second approach we want to discuss is the usage of an exponential function given by the system's potential $U(r) = 0.5 \cdot (x - a)^2$ for the radial distribution function. This is subject to the next subsection.

Exponential Ansatz

When using for fixed $a = 1$ the mapping $g_{exp} : \mathbf{r} \mapsto \exp(-u_a(\mathbf{r})) = \exp(-(||\mathbf{r}||_2 - a)^2/2)$ for the radial distribution function, the static structure factor S_* is calculated via

$$\begin{aligned} S_*(\mathbf{q}) &= 1 + \rho_* \cdot \int_{\mathbb{R}^3} (g_{exp}(\mathbf{r}) - 1) \cdot \exp(i \cdot \mathbf{r} \cdot \mathbf{q}) \lambda(d\mathbf{r}) \\ &= 1 + \rho_* \cdot 4\pi \cdot \int_{\mathbb{R}_{>0}} (g_{exp,||}(r) - 1) \cdot r^2 \cdot \text{sinc}(r \cdot |\mathbf{q}|) \lambda(dr), \end{aligned}$$

which can be validated by equation (28). With this change in the integrand, the behaviour of S_* with regard to ρ_* is also altered. One can see in direct comparison with the model calculated by the OZ equation that the exponential ansatz yields less physical meaningful results. Its range of validity is limited to small densities, as figure 18 suggests.

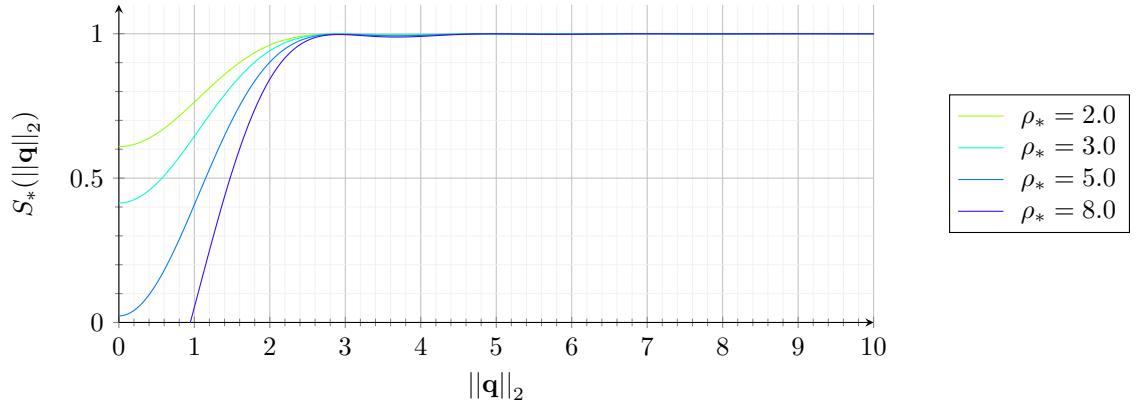
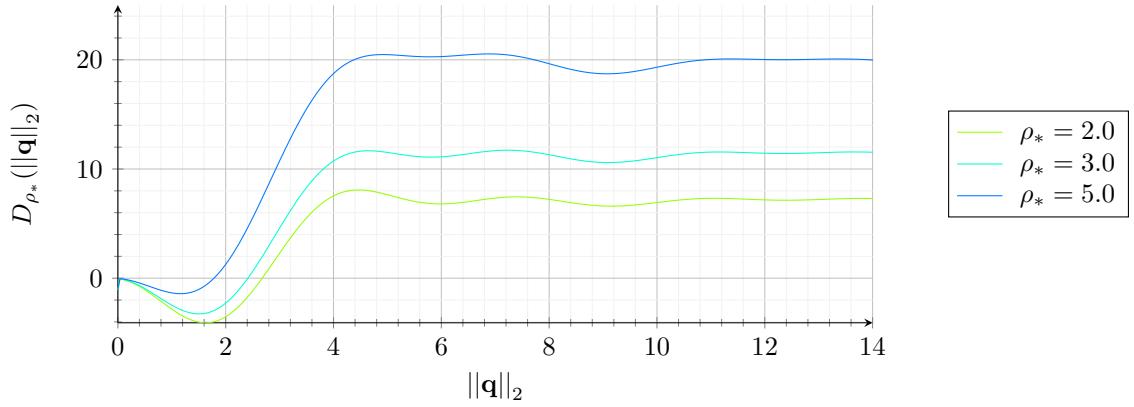
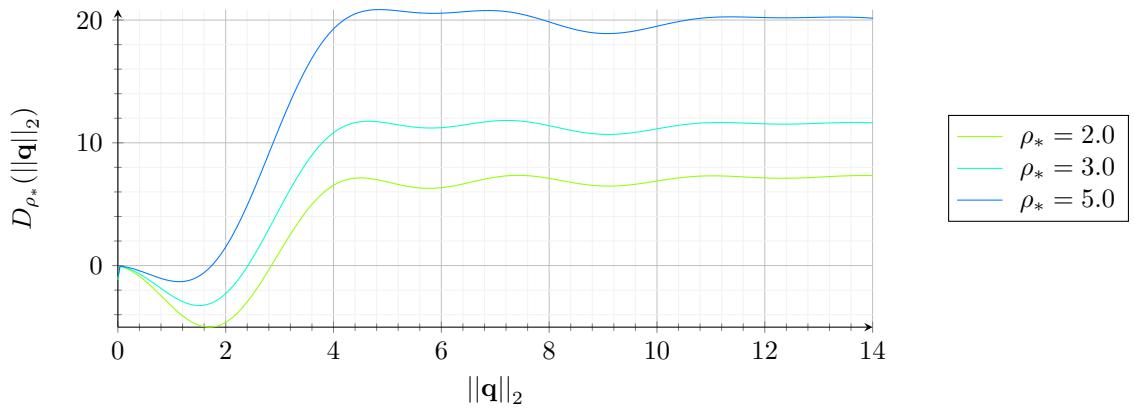


Figure 18: Altered formula for $S_*(q) = 1 + \rho_* \cdot \mathcal{F}(g_{exp} - 1)(q)$ for different densitys ρ_* .

With the gaussian based structure factor we can now take a look at the resulting dispersion functions. Within physical range we find again very similar results, as one can see in figure 19.



(a) The structure factor is set to $S_*(q) = 1.0$ for all densitys.



(b) The structure factor is set to $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}(g_{exp} - 1))(q)$ for all densitys.

Figure 19: The dispersion relation D_{ρ_*} for small densitys ρ_* .

In comparison with eachother using the difference method we find similar results as above for the densities 2.0 and 3.0, but an inverted behaviour for $\rho_* = 5.0$, as figure 20 shows.

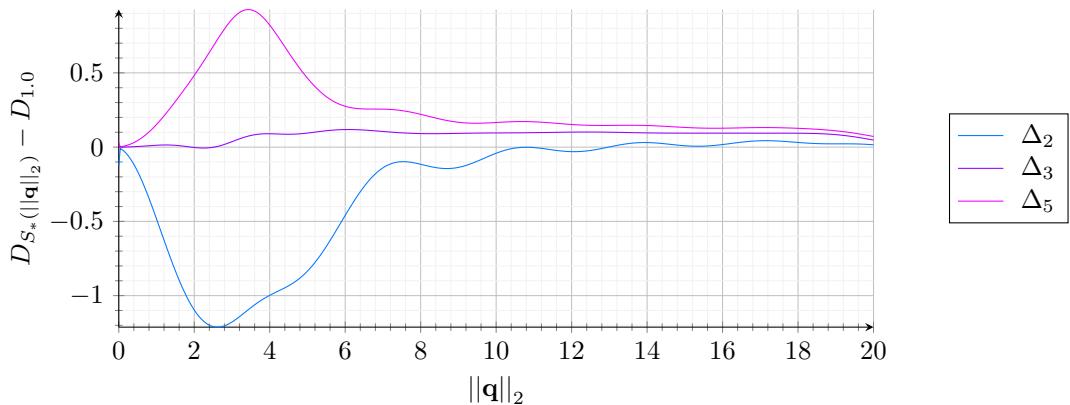


Figure 20: Comparison of the dispersion relation D_{ρ_*} for $\rho_* = 5.0$ with $S_*(q) = 1.0$ and $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}g_{gau} - 1.0)(q)$. It is drawn $D_{S_*(q)} - D_{1.0}$ for $D_{S_*(q)}$ the dispersion relation with the corrected structure factor. A positive value means that dispersion with static structure factor yields a higher amplitude.

For the velocity of sound using the same methods as above we have again a similar behaviour without structure factor correction, see figure 21.

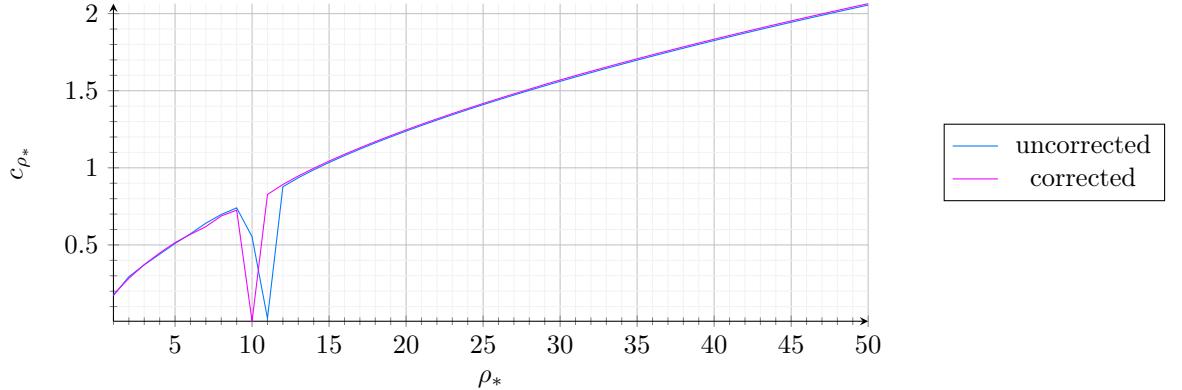


Figure 21: The velocity of sound c_{ρ_*} for different densities ρ_* in comparison with $S_*(q) = 1.0$ and $S_*(q) = 1.0 + \rho_* \cdot (\mathcal{F}(g_{exp} - 1))(q)$. Using the exponential ansatz for the radial distribution function.

Lastly in our investigation we found an interesting periodic behaviour for $\rho_* = 10.0$ in the exponential ansatz, see figure 22. Another interesting behaviour has been noticed at $\rho = 11.0$ with respect to convergence issues.

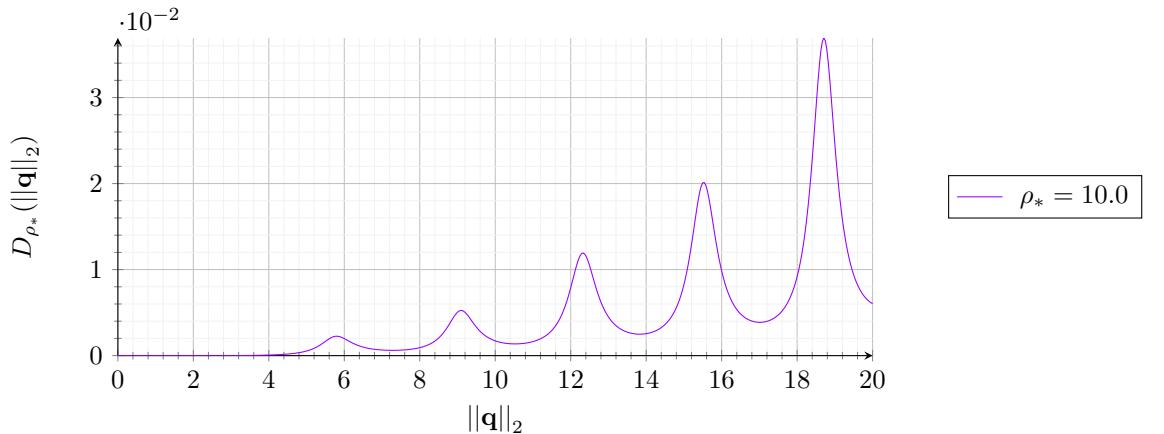


Figure 22: Interesting periodic behavior for the exponential ansatz at $\rho_* = 10.0$.

A note to a Code Mistake

During the final review of the numerical analysis section of this thesis, a mistake in the code was discovered. The mistake was made in the calculation of the static structure factor $S_*(q)$ and within the definition of its Fourier transformation. In the Code version that was used to produce the data for this thesis, unfortunately the square of the density ρ_* was multiplied with the integrand, instead of the Jacobian determinant factor of r^2 . This lead to the wrong implementation:

```

1 cFT_integrand = (q,r) -> 2 * sinc(q * r)
2 cFT = q -> sum([\color{red}\rho^2\color{black} * 2 * pi * gm * x * Δr
    for (x,gm) in zip(cFT_integrand.(q, solution.r),[x - 1 for x in
    solution.gr]))])

```

Correcting this mistake, the code should look like this:

```

1 cFT = q -> begin
2     if exp_g_toggle
3         sum(r^2 * 2 * pi * (exp(-1 * Uf(r, params)) - 1) * x
4             * Δr for (x,r) in zip(cFT_integrand.(q, solution
5                 .r),solution.r)))
6     else
7         sum([r^2 * 2 * pi * gm * x * Δr for (x,gm,r) in zip(
8             cFT_integrand.(q, solution.r),[x - 1 for x in
9                 solution.gr],solution.r)]) # use cFT_integrand on
10                all r values from solution.r, then discretely
11                integr.
12
13 end
14 end

```

Notice that this mistake also affects the calculation of the exponential ansatz for the radial distribution function. *However*, the results presented in this thesis are based on the corrected implementation, which was used for the final re-evaluation of the data. The results presented in this thesis are therefore not affected by this mistake.

↪ CONCLUSION AND OUTLOOK ↵

Chapter 5

In this thesis we have been able to build a foundation of ERM for preparation of the position probability correction. Using first order perturbation theory, the corresponding Feynman rules have been derived and the self consistent Born approximation has been calculated explicitly.

Following the thesis's main goal, the static structure factor S_* has been introduced as $S_*(\mathbf{q}) = 1 + \rho_* \cdot \frac{(\mathcal{F}g_0 - 1)(\mathbf{q})}{\hat{\delta}\rho_{R_\omega}(\mathbf{q}) \cdot \hat{\delta}\rho_{R_\omega}(-\mathbf{q})}$ and brought to relation with the expected value of the density fluctuations via $\hat{\delta}\rho_{R_\omega}(\mathbf{q}) \cdot \hat{\delta}\rho_{R_\omega}(-\mathbf{q}) = S_*(\mathbf{q})/\rho_*$. Accordingly, the Feynman rules have been corrected to include the static structure factor in the one loop order. The corrected self energy $\Sigma_{S_*}^{(1)}$ used in the Dyson fixed point equation has been derived to

$$\Sigma_{S_*}^{(1)} = \frac{1}{\rho_*} \cdot \int_{\mathbb{R}^d} S_*(\mathbf{q}) \cdot G(p - \mathbf{q}, z) \cdot V(\mathbf{q}, p)^2 \lambda(d\mathbf{q}).$$

Numerical analysis of the stated analytical model have been performed on a Heaviside spring function $f_a^{(\text{num})}(r) = \mathbb{1}_{\mathbb{R}_{<a}}(r)$ in a three dimensional space with the pair potential $u(r) = (r - a)^2/2$. For the calculation of the static structure factor we have used the hypernetted chain approximation, the initial guess for the dyson equation was set to the bare propagator $G_0(\mathbf{q}) = (z - \rho_* \cdot (\hat{F}_a(0) - \hat{F}_a(\mathbf{q})))^{-1}$. By setting $z = 0$ we have been able to calculate the Dispersion relation under consideration of S_* . The values of S_* have been entirely positive for all tested densities. For small wave vector norms we conclude a decrease in compressibility due to the steep decline of S_* . The speed of sound however is shown to be nearly unchanged for all densities. Also a general difference between the dispersion relation amplitudes of the corrected and uncorrected model has been observed to decrease with increasing density.

Numerical analysis of gaussian g_{exp} as the radial distribution showed similar results. It has been shown that small densities overall tend to numerical instability in both models.

A brief outlook on handling correlators of $\hat{\delta}\rho$ functions has been given based on Crooks and Chandler in [17]. This could be a promising approach to further investigate higher loop orders and to further enhance research on the ERM model under consideration of correlated disorder.

Overall we have seen that implementation of the equilibrium structure factor S_* in the ERM model has no significant impact on the dispersion relation. If a non-equilibrium theory however brings significant changes to the dispersion relation is subject to further research.

Appendix

↪ MISSED PROOFS ↵

During the derivation of the Green's function or resolvent of our system's Laplace matrix we needed the Laplace transform of the second derivative with respect to time of a Laplace transformable function f . For this we generally stated $(\mathcal{L}f^{(n)})(s) = s^n \cdot (\mathcal{L}f)(s) - \sum_{k=0}^{n-1} s^{n-1-k} \cdot f^{(k)}(0)$, which for every $n \in \mathbb{N}$ and $f \in C^n(\mathbb{R}_{>0})$ of exponential order we now need to prove.

Proof (of Lemma 1). We start by induction. For $n = 1$ using partial integration we have

$$(\mathcal{L}f)(s) = \int_{\mathbb{R}_{>0}} f'(t) \cdot e^{-st} \lambda(dt) = [f \cdot e^{-s \cdot}]_0^\infty - \int_{\mathbb{R}_{>0}} f(t) \cdot \frac{d}{dt} e^{-st} \lambda(dt).$$

Because of $\lim_{x \rightarrow \infty} f(x) \cdot e^{-sx} = 0$ and $f(0) \cdot e^0 = f(0)$, as well as $\frac{d}{dt} e^{-st} = -s \cdot e^{-st}$ we therefore get

$$(\mathcal{L}f)(s) = -f(0) \cdot 1 + s \cdot \int_{\mathbb{R}_{>0}} f(t) \cdot e^{-st} \lambda(dt) = -f(0) + s \cdot \mathcal{L}f(s).$$

For the induction step we assume the statement to hold for $n \in \mathbb{N}$ and show it for $n+1$. By again partially integrating we find

$$(\mathcal{L}f^{(n+1)})(s) = \int_{\mathbb{R}_{>0}} f^{(n+1)}(t) \cdot e^{-st} \lambda(dt) = [f^{(n)} \cdot e^{-s \cdot}]_0^\infty - \int_{\mathbb{R}_{>0}} f^{(n)}(t) \cdot \frac{d}{dt} e^{-st} \lambda(dt).$$

As discussed above we see $[f^{(n)} \cdot e^{-s \cdot}]_0^\infty = -f^{(n)}(0)$, which gives

$$(\mathcal{L}f^{(n+1)})(s) = -f^{(n)}(0) + s \cdot \mathcal{L}f^{(n)}(s).$$

By the induction hypothesis we can insert the expression for $\mathcal{L}f^{(n)}(s)$ and obtain

$$\begin{aligned} (\mathcal{L}f^{(n+1)})(s) &= -f^{(n)}(0) + s \cdot \left(s^n \cdot (\mathcal{L}f)(s) - \sum_{k=0}^{n-1} s^{n-1-k} \cdot f^{(k)}(0) \right) \\ &= s^{n+1} \cdot (\mathcal{L}f)(s) - \sum_{k=0}^n s^{n-k} \cdot f^{(k)}(0). \end{aligned}$$

This concludes the proof. q.e.d.

Proof. The Fourier Transform $\mathcal{F}F_a$ of F_a in three dimensions is given by

$$(\mathcal{F}F_a)(\mathbf{q}) = \int_{\mathbb{R}^3} F_a(\mathbf{r}) \cdot e^{i \cdot \langle \mathbf{r}, \mathbf{q} \rangle} \lambda(d\mathbf{r}),$$

while radial symmetry of $F_a = H_a \circ ||\cdot||_2$ suggests a spherical transformation. Using $(\rho, \vartheta, \varphi) \mapsto \rho \cdot (\sin(\vartheta) \cdot \cos(\varphi), \sin(\vartheta) \cdot \sin(\varphi), \cos(\vartheta))$ with the Jacobian absolute determinant

$(\rho, \vartheta) \mapsto \rho^2 \cdot \sin(\vartheta)$ we get

$$\int_{(-\pi, \pi)} \int_{\mathbb{R}_{>0}} \int_{[0, \pi)} H_a(\rho) \cdot \exp(\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta)) \cdot \rho^2 \cdot \sin(\vartheta) \lambda^3(d(\vartheta, \rho, \varphi)).$$

Again we can use the differentiation technique to evaluate the inner integral to

$$\int_{[0, \pi)} \frac{\overset{\circ}{i}}{\rho \|\mathbf{q}\|_2} \cdot \frac{d}{d\vartheta} \exp(-\overset{\circ}{i} \rho \cdot \|\mathbf{q}\|_2 \cdot \cos(\vartheta)) \lambda(d\vartheta) = \frac{\overset{\circ}{i} \cdot (\exp(-\overset{\circ}{i} \rho \cdot \|\mathbf{q}\|_2) - \exp(\overset{\circ}{i} \rho \cdot \|\mathbf{q}\|_2))}{\rho \cdot \|\mathbf{q}\|_2}.$$

The outer integral on $(-\pi, \pi)$ yields a factor of 2π due to independence of φ , which leaves us one last integral to solve:

$$(\mathcal{F}F_a)(\mathbf{q}) = 2\pi \overset{\circ}{i} \cdot \|\mathbf{q}\|_2^{-1} \cdot \int_{\mathbb{R}_{>0}} H_a(\rho) \cdot (\exp(-\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2) - \exp(\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2)) \cdot \rho \lambda(d\rho).$$

The boundary condition of $H_a = \mathbb{1}_{[0, a]}$ suggests a smaller integration domain $[0, a)$ for the integral, so that for $g(\rho) := \exp(-\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2) - \exp(\overset{\circ}{i} \cdot \rho \cdot \|\mathbf{q}\|_2)$ we can compute the integral using integration by parts to

$$\int_{[0, a]} g(\rho) \cdot \rho \lambda(d\rho) = [G(\rho) \cdot \rho]_0^a - \int_{[0, a]} G(\rho) \lambda(d\rho)$$

Here we used the notation G for the first anti-derivative of g . Evaluating $G(\rho) := \int_{[0, \rho]} g \lambda$, as well as $\int_{(0, a)} G \lambda$ we find the result

$$\begin{aligned} (\mathcal{F}F_a)(\mathbf{q}) &= \frac{2\pi \overset{\circ}{i}}{\|\mathbf{q}\|_2} \cdot \frac{2 \cdot (a \cdot \cos(a \cdot \|\mathbf{q}\|_2) \cdot \|\mathbf{q}\|_2 - \sin(a \cdot \|\mathbf{q}\|_2))}{\|\mathbf{q}\|_2^2} \cdot \overset{\circ}{i} \\ &= 4\pi \cdot \frac{\sin(a \cdot \|\mathbf{q}\|_2) - a \cdot \|\mathbf{q}\|_2 \cdot \cos(a \cdot \|\mathbf{q}\|_2)}{\|\mathbf{q}\|_2^3}. \end{aligned}$$

We now need to investigate $\lim_{r \rightarrow 0} (\mathcal{F}F_a)(B_r(0))$.

$$\begin{aligned} &\left(\frac{4\pi}{\|\mathbf{q}\|_2^3} \right) \cdot \left(\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} \cdot (a \cdot \|\mathbf{q}\|_2)^{2n+1} - a \cdot \|\mathbf{q}\|_2 \cdot \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} \cdot (a \cdot \|\mathbf{q}\|_2)^{2n} \right) \\ &= 4\pi \cdot \left(\sum_{n=0}^{\infty} \frac{(-1)^n \cdot a^{2n+1}}{(2n+1)!} \|\mathbf{q}\|_2^{2n-2} - a \cdot \|\mathbf{q}\|_2 \cdot \sum_{n=0}^{\infty} \frac{(-1)^n \cdot a^{2n}}{(2n)!} \cdot \|\mathbf{q}\|_2^{2n-3} \right) \\ &= 4\pi \cdot \left(\sum_{n=0}^{\infty} \frac{(-1)^n \cdot a^{2n+1}}{(2n+1)!} \cdot \|\mathbf{q}\|_2^{2n-2} - \frac{(-1)^n \cdot a^{2n+1}}{(2n)!} \cdot \|\mathbf{q}\|_2^{2n-2} \right) \end{aligned}$$

Lets take a closer look at the sum (equal to the *Laurent series* at $z_0 = 0$) and its critical summand at $n = 0$, where most factors vanish to one:

$$a^2 \cdot \|\mathbf{q}\|_2^{-2} - a^2 \cdot \|\mathbf{q}\|_2^{-2} = 0.$$

This means the singularity at $\mathbf{q} = 0$ vanishes. Furthermore it can be removed with a

constant factor $a^3/3$ arising from the next summand at $n = 1$:

$$\begin{aligned} & \left(\frac{-1 \cdot a^3}{3!} - \frac{-1 \cdot a^3}{2!} \right) + \sum_{n=2}^{\infty} \frac{(-1)^n \cdot a^{2n+1}}{(2n+1)!} \cdot \|\mathbf{q}\|_2^{2n-2} - \frac{(-1)^n \cdot a^{2n+1}}{(2n)!} \cdot \|\mathbf{q}\|_2^{2n-2} \\ &= \left(\frac{1 \cdot a^3}{3} \right) + \sum_{n=2}^{\infty} \frac{(-1)^n \cdot a^{2n+1}}{(2n+1)!} \cdot \|\mathbf{q}\|_2^{2n-2} - \frac{(-1)^n \cdot a^{2n+1}}{(2n)!} \cdot \|\mathbf{q}\|_2^{2n-2}. \end{aligned}$$

Notice that for $\mathbf{q} = 0$ now the leftover sum vanishes to 0 and the remainder $a^3/3$ arises. With the full definition of $\mathcal{F}F_a$ we therefore found

$$(\mathcal{F}F_a)(\mathbf{q}) = \begin{cases} 4\pi \cdot (\sin(a \cdot \|\mathbf{q}\|_2) - a \cdot \|\mathbf{q}\|_2 \cdot \cos(a \cdot \|\mathbf{q}\|_2)) \cdot \|\mathbf{q}\|_2^{-3} & \mathbf{q} \neq 0, \\ 4\pi \cdot a^3/3 & \mathbf{q} = 0. \end{cases}$$

This concludes the proof.

q.e.d.

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↪ CODE ↵

The code used in this project is publicly available on GitHub. The repository can be found at

<https://github.com/unb3rechenbar/BA24-CorDis.git>

Please do not hesitate to contact me in case of any problems or questions.

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