Scattering amplitudes from spectral densities

An Haag-Ruelle based approach to scattering theory, suitable for lattice applications.

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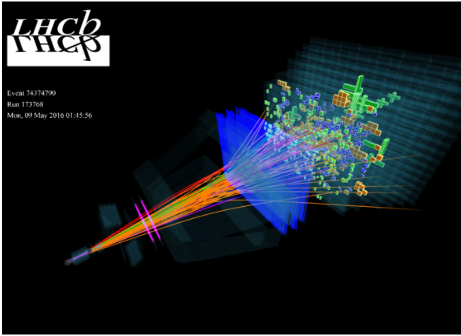
Overview of the presentation

- Introduction: general aspects of scattering theory.
- Definition and properties of the spectral density.
- Haag-Ruelle scattering theory: relation between S-matrix element and spectral density.
- Perturbative tests
- State of the art of the numerical algorithms
- Conclusions



General aspects of scattering theory

- The final goal of a calculation in Scattering theory is the detailed comprehension of a collision experiment.
- The widely used formulation of the S-matrix is the LSZ-reduction formula, extremely powerful tool in perturbation theory:

$$S_{p'_1,\ldots,p'_m;p_1,\ldots,p_n} =_{out} \langle p'_1,\ldots,p'_m| \, |p_1,\ldots,p_n\rangle_{in} =$$

$$= \prod_{i,j} \frac{(p_i'^2 - m^2)(p_j^2 - m^2)}{Z_i Z_j} \int d^4x'_i d^4x_j e^{i\sum p'_i \cdot x'_i - i\sum p_j \cdot x_j}.$$

$$\cdot T \langle 0| \, \phi(x'_m)\ldots\phi(x_1) \, |0\rangle$$

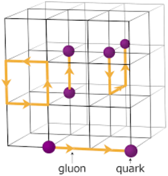
Where $Z_i = \langle 0| \, \phi \, |k_{i,in}\rangle$. So the probability amplitude is the Fourier-transform of the correlator, with the amputation of the external lines.

General aspects of scattering theory

- Unfortunately this is not the end of the story. The extraction of observable quantities it isn't reliable in a regime in which it's not possible to use perturbation theory.
- The only well-known approach to extract time-ordered correlators in a non-perturbative way is the Lattice. But there are two main problems:
    1. The evolution is in Euclidean time:

    $$O(x) = e^{Ht} O(\vec{x}) e^{-Ht}$$

    2. The volume is finite



Definition of the spectral density

Let's analyze the structure of the Correlator $C(\{x\}) = T \langle 0| O_n(x_n) \dots O_1(x_1) |0\rangle$ in Euclidean and Minkowsky time. Inserting n-times the identity $1 = \int d^4p\, \delta^4(\hat{P} - p)$:

- In Minkowskian time:

$$C(\{x\}) = \int d^4p_i\, \theta(t_{i+1} - t_i) \dots e^{-i(p_i^0 t_i - \vec{p}_i \cdot \vec{x}_i)} \dots \langle 0| O_n \delta^4(\hat{P} - p_n) \dots O_2 \delta^4(\hat{P} - p_1) O_1 |0\rangle$$

- In Euclidean time:

$$C(\{x\}) = \int d^4p_i\, \theta(t_{i+1} - t_i) \dots e^{-(p_i^0 t_i) + i(\vec{p}_i \cdot \vec{x}_i)} \dots \langle 0| O_n \delta^4(\hat{P} - p_n) \dots O_2 \delta^4(\hat{P} - p_1) O_1 |0\rangle$$

The green quantity is the same in the two formalism! It is the so-called spectral density.

Definition of the spectral density

We have seen that the spectral density is the same in the Minkowskian and Euclidean time

$$\rho(\{p\}) = \langle 0| O_n \delta^4(\hat{P} - p_n) \dots O_2 \delta^4(\hat{P} - p_1) O_1 |0\rangle$$

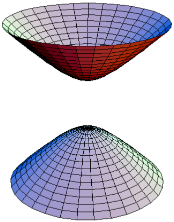
In the rest of this presentation the working hypotesis is that ρ can be computed on the lattice. This is only partially true.
But if we find the relation between the spectral density and the S-matrix in a rigorous way, it would be possible to extract directly S-matrix elements from non-perturbative lattice-calculations.

Haag-Ruelle approach

The first step to build asymptotic states is the definition of **semi-local operators**:

$$\phi_\varepsilon(x) = \int d^4y\, \Sigma_\varepsilon(y-x)\phi(y)$$

$\Sigma_\varepsilon(y-x)$ is a smearing function, centered around the single-particle hyperboloid, with compact support and rapidely decreasing.



$$\Sigma_\varepsilon(y-x) = \int \frac{d^4p}{(2\pi)^4} e^{-ip\cdot(y-x)}\Sigma_\varepsilon(p)$$

$$\Sigma_\varepsilon(p) = \begin{cases} 0, & |p^2-m^2| > \varepsilon \\ 1, & p^2 = m^2 \end{cases}$$

Haag-Ruelle approach

Now we build the interpolating operators performing the convolution between the semi-local operator and a solution of the Klein-Gordon equation:

$$O_\varepsilon(t,\vec{k}) = \int d^3x \psi(x,\vec{k})\phi_\varepsilon(x) \quad \psi(x,\vec{k}) = \int \frac{d^3q}{(2\pi)^3}\frac{e^{-i(t\omega(\vec{q})-\vec{x}\cdot\vec{q})}}{2\omega(\vec{q})}\tilde{\psi}(q,\vec{k})$$

Fourier-transforming ψ and ϕ we have the useful expression

$$O_\varepsilon(t,\vec{k}) = \int \frac{d^4q}{(2\pi)^4} e^{it\left[H-q-\omega(\vec{P}-\vec{q})\right]}\Delta_\varepsilon(P-q,\vec{k})\phi(2\pi)^4\delta^4(P-q)$$

$\Delta_\varepsilon(P-q,\vec{k})$ is simply the product between the rapidely-decreasing function Σ_ε and the wave-packet, so it has the same behaviour of Σ_ε.

Haag-Ruelle approach

Now we can act on the vacuum with the interpolating operators:

$$O_\varepsilon(t,\vec{k})\,|0\rangle = e^{it\left[H-\omega(\vec{P})\right]}\Delta_\varepsilon(P,\vec{k})\phi\,|0\rangle$$

Now, using the property that $\Delta_\varepsilon(P-q,\vec{k})$ has support only on the Hamiltonian spectrum, $H=\sqrt{m^2+\vec{P}^2}=\omega(\vec{P})$, so:

$$O_\varepsilon(t,\vec{k})\,|0\rangle = \Delta_\varepsilon(P,\vec{k})\phi\,|0\rangle = \int \frac{d^3p}{(2\pi)^3}\,|\vec{p}\rangle_{in}\,\frac{{}_{in}\langle\vec{p}|\,\phi\,|0\rangle}{2\omega(\vec{p})}\psi(\vec{p},\vec{k})$$

How to build n-particle states? Applying n-times O_ε on the vacuum. But now the time-dependence is not trivial!

$$O_\varepsilon(t_n,k_n)\ldots O_\varepsilon(t_1,\vec{k}_1)\,|0\rangle$$

Haag-Ruelle approach

It is possible to show that the following limit converges to the asymptotic n-particle state: [1] [2] [3]

Asymptotic states from Interpolating Operators

$$\lim_{t_1 \to -\infty} \dots \lim_{t_n \to -\infty} O_\varepsilon(t_n, \vec{k}_n) \dots O_\varepsilon(t_1, \vec{k}_n) |0\rangle =$$

$$= \int \prod_i \frac{d^3 p_i}{(2\pi)^3} \frac{Z_i \psi(\vec{p}_i, \vec{k}_i)}{2\omega(\vec{p}_i)} |\vec{p}_n, \dots, \vec{p}_1\rangle_{in}$$

[1] Haag, R. (1955). On quantum field theories. Kgl. Danske Videnskab. Selskab, Mat.- Fys. Medd., 29, 1–37.

[2] Haag, R. (1992). Local Quantum Physics (1st edn). Springer-Verlag, Berlin.

[3] Ruelle, D. (1962). On the asymptotic condition in quantum field theory. Helvetica Physica Acta, 35, 147–163.

S-matrix element

Finally, we can find the relation between the S-matrix element and the spectral density doing the braket between two asymptotic states.
For a $n \to m$ S-matrix element:

$$\mathrm{S}_{m,n}(\{k\},\{\bar{k}\}) = \lim_{t_1\to\infty}\ldots\lim_{t_n\to\infty}\lim_{\bar{t}_1\to+\infty}\ldots\lim_{\bar{t}_m\to+\infty} S_{m,n}(\{-t\},\{\bar{t}\},\{k\},\{\bar{k}\})$$

$$S_{m,n}(\{-t\},\{\bar{t}\},\{k\},\{\bar{k}\}) = \int\left[\prod_{j=1}^{n}\frac{d^4q_j}{(2\pi)^4}\frac{e^{-it_j(q_j^0-\omega(\vec{q}_j))}\Delta_\varepsilon(q_j,\vec{k}_j)2\omega(\vec{k}_j)}{Z_j}\right]$$
$$\left[\prod_{i=1}^{m}\frac{d^4\bar{q}_i}{(2\pi)^4}\frac{e^{-i\bar{t}_i(\bar{q}_i^0-\omega(\vec{\bar{q}}_i))}\Delta_\varepsilon(\bar{q}_i,\vec{\bar{k}}_i)2\omega(\vec{\bar{k}}_i)}{Z_i^*}\right](2\pi)^4\delta^4\left(\sum_{i=1}^{m}\bar{q}_i-\sum_{j=1}^{n}q_j\right)\rho(\bar{q}_{1,\ldots,m-1},q_{1,\ldots,n})$$

Other useful expressions of the S-matrix element

We want to get rid of the time-dependence in the previous formula using the identity

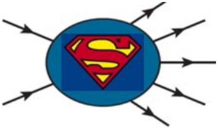
$$\theta(t)e^{-iqt} = \int_{-\infty}^{+\infty} dp \frac{sin(pt)}{\pi p} \frac{p}{p+q-i\varepsilon} = \int_{-\infty}^{+\infty} dp \frac{\delta_{\frac{1}{t}}(p)p}{p+q-i\varepsilon}.$$

The function $\delta_{\frac{1}{t}}$ is a Dirac-δ function approximation in the limit in which $t \to \infty$. So in this limit we can use another δ approximating function as

$$\delta_\sigma(p) = \frac{\sigma}{\pi(p^2+\sigma^2)}$$

Other useful expressions of the S-matrix element

- New smearing parameter σ
- Haag-Ruelle smearing functions Δ_ε
- δ^4 of energy-momentum conservation



$$S_{m,n}(\{k\},\{\bar{k}\}) = \lim_{\bar{\sigma}_i\sigma_j\to 0}\int\prod_j \frac{d^4q_j}{(2\pi)^4}\,\frac{(-i\sigma_j)2\omega(\vec{k}_j)\Delta_\varepsilon(q_j,\vec{k}_j)}{Z_j\left[\sum_{b=1}^{j}(q_b^0-\omega(\vec{q}_b))-i\sigma_j\right]}\cdot$$

$$\cdot\int\prod_i \frac{d^4\bar{q}_i}{(2\pi)^4}\,\frac{(-i\bar{\sigma}_i)2\omega(\vec{k}_i)\Delta_\varepsilon(\bar{q}_i,\vec{k}_i)}{Z_i^*\left[\sum_{a=1}^{i}\left(\bar{q}_a^0-\omega(\vec{\bar{q}}_a)\right)-i\bar{\sigma}_i\right]}\cdot$$

$$\cdot\int\frac{d^4\bar{q}_m d^4q_n}{(2\pi)^8}\,\frac{(-i\sigma_n)(2\pi)^4\delta^4\left(\sum_{i=1}^{m}\bar{q}_i-\sum_{j=1}^{n}q_j\right)\Delta_\varepsilon(\bar{q}_m,\vec{\bar{k}}_m)\Delta_\varepsilon(q_n,\vec{k}_n)\rho(\bar{q}_1,\ldots,\bar{q}_m;q_1,\ldots,q_n)}{\sum_{b=1}^{n}(q_b^0-\omega(\vec{q}_b))+\sum_{a=1}^{m}(\bar{q}_a^0-\omega(\vec{\bar{q}}_a))-i\sigma_n}$$

Perturbative tests

To test the formulae given above, perturbative calculations were performed.
The main problem is that Feynmann diagrams are tailor-made to calculate time-ordered correlators, not spectral densities!

$$\rho(p_1, \ldots, p_n) = \int d^4x_i \, e^{ix_i p_i} \ldots \langle 0| \phi(x_1) \ldots \phi(x_n) |0\rangle$$

$$\mathcal{C}(p_1, \ldots, p_n) = \int d^4x_i \, e^{ix_i p_i} \ldots T \, \langle 0| \phi(x_1) \ldots \phi(x_n) |0\rangle$$

The calculations followed several steps:

1. Select the process that we want to analyze ($1 \rightarrow 2$)
2. Calculate ρ explicitly (non-trivial result on its own)
3. Extraction of the S-matrix elements with the formulae given before.

Perturbative tests: spectral density at tree level of a 2 point correlation function

The starting point is the correlator:

$$C(t) = \theta(t)\langle 0|\,\phi(\vec{x},t)\phi(0)\,|0\rangle + \theta(-t)\langle 0|\,\phi(0)\phi(\vec{x},t)\,|0\rangle = C_+(t) + C_-(t)$$

It is important to notice that

$$\theta(t)C(t) = C_+(t) = \int \frac{d^3q}{(2\pi)^3} e^{iq\cdot x} \int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi}\theta(t)e^{-i\omega_1 t}\rho(\omega_1)$$

Fourier-transforming everything

$$\tilde{C}(\vec{k}, k^0 + i\varepsilon) = i\int_{-\infty}^{+\infty} \frac{d\omega_1}{2\pi} \frac{\rho(\omega_1)}{k^0 - \omega_1 + i\varepsilon}$$

So ρ is simple to find:

$$\rho(k^0) = \lim_{\varepsilon\to 0} \tilde{C}(k^0 + i\varepsilon) - \tilde{C}(k^0 - i\varepsilon)$$

Perturbative tests: spectral density at tree level of a 2 point correlation function

On the other hand, $\tilde{C}(k^0 + i\varepsilon)$ is computable with the Feynmann diagrams in perturbation theory. So, in the case of the 2-point correlation function:

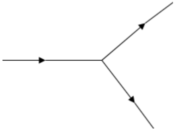
$$\tilde{C}(k^0 + i\varepsilon) = \int d^3x \, e^{-i\vec{k}\cdot\vec{x}} \int_{-\infty}^{+\infty} dt e^{i(k^0+i\varepsilon)t} \theta(t) C_+(t) =$$

$$= \cdots = i \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{(2\pi)\delta(E-\omega)}{2\omega(k^0 - \omega + i\varepsilon)}$$

Finally, the spectral density is

$$\rho(\omega) = \frac{2\pi\delta(E-\omega)}{2\omega}$$

Perturbative tests: $\lambda\phi^3$



$$\mathcal{C}(q_1,q_2) = \frac{\lambda}{[(q_1+q_2)^2-M^2+i\varepsilon]\left[q_1^2-m^2+i\varepsilon\right]\left[q_2^2-m^2+i\varepsilon\right]}$$

$$\rho(q_1,q_2) = \frac{\lambda(2\pi)^2}{4\omega_1\omega_2}\frac{\delta(q_1^0+q_2^0-\omega_1-\omega_2)\delta(q_1^0-\omega_1)}{[(\omega_1-\omega_2)^2-\Omega^2](1-i\varepsilon)}+$$

$$+\frac{\lambda(2\pi)^2}{4\omega_1\Omega}\frac{\delta(q_1^0+q_2^0-\Omega)\delta(q_1^0-\omega_1)}{\left[(\Omega-\omega_1)^2-\omega_2^2\right](1-i\varepsilon)}+$$

$$+\frac{\lambda(2\pi)^2}{4\omega_2\Omega}\frac{\delta(q_1^0+q_2^0-\Omega)\delta(q_1^0-\Omega-\omega_2)}{\left[(\Omega+\omega_2)^2-\omega_1^2\right](1-i\varepsilon)}$$

Selecting the process in which $\Omega = \omega_1 + \omega_2$:

$$S = \lambda \int \frac{d^3q_1}{(2\pi)^3}\frac{d^3q_2}{(2\pi)^3}\psi_\varepsilon^*(\vec{q}_1+\vec{q}_2)\psi_\varepsilon(\vec{q}_1)\psi_\varepsilon(\vec{q}_2)(2\pi)\,\delta(\Omega-\omega_1-\omega_2)$$

Numerical extraction of ρ

In order to extract ρ from the lattice there are a lot of problems to solve:

1. Performing an inverse Laplace-transorm

$$C(t) = \int_0^{+\infty} dE\, \rho_L(E) e^{-tE}$$

2. The simulation is performed at finite volume $\rightarrow$ the spectrum is discrete!

But with the Haag-Ruelle smearing the problem can be faced! On the lattice it is possible to calculate directly the smeared spectral density

$$\hat{\rho}_L(\sigma, E_*) = \int_0^{+\infty} dE\, \rho_L(E) \Delta_\sigma(E, E_*)$$

Numerical algorithm

On the lattice we have a finite temporal extent, so the correlator will be:

$$C(t) = \int_0^{+\infty} dE\, \rho(E) b_T(t, E)$$

Where $b_T(t, E) \to e^{-tE}$ for $T \to \infty$.
Given an input smearing-function $\Delta_\sigma(E_*, E)$ (for example a Gaussian), we can search for an approximation of this Δ_σ that lives in the space spanned by the basis-functions

$$\bar{\Delta}_\sigma = \sum_{t=0}^{t_{max}} g_t(\lambda, E_*) b_T(t, E)$$

It is possible to demonstrate that the smeared spectral density is recovered by

$$\hat{\rho}_L(\sigma, E_*) = \sum_{t=0}^{t_{max}} g_t(\lambda, E_*) C(t+1)$$

Numerical algorithm

In order to determine g_t, we have to minimize the functional

$$W[\lambda, g] = (1-\lambda)A[g] + \lambda B[g]$$

In this equation, $A[g]$ is the deterministic part, that represents the distance between Δ and $\bar{\Delta}$:

$$A[g] = \int_{E_0}^{+\infty} dE \, |\bar{\Delta}_\sigma(E_*, E) - \Delta_\sigma(E_*, E)|^2$$

While $B[g]$ is a functional that quantifies the statistical error.
λ is a free parameter in this convex combination, but if we see W as a **function of** λ, we can take the λ^* in which W has the maximum value (it exists, but it may not be unique).
In the ideal case in which $t_{max} \to \infty$, the error in the approximation goes to zero.

Numerical algorithm

During the minimization of the functional $W[\lambda, g]$ we need to evaluate the integral

$$f_t(E_*) = \int_0^\infty dE\, b_T(t+1, E)\Delta_\sigma(E_*, E)$$

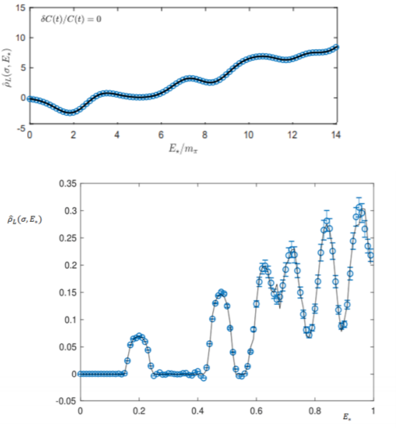
If Δ_σ is a function with compact-support, as the one in Haag-Ruelle scattering theory, we can approximate $f_t(E_*)$ with Gauss-Chebyshev polynomials:

$$f_t = \sigma e^{-t x_0} \lim_{N\to\infty} \frac{\pi}{N} \sum_{i=1}^{N} g_{t\sigma}(x_i^N)$$

Where

$$g_{t\sigma}(x) = e^{-\frac{1}{1-x^2} t\sigma x}, \qquad x_i^N = \cos\left[\frac{\pi}{N}\left(i - \frac{1}{2}\right)\right]$$

Numerical extraction of ρ



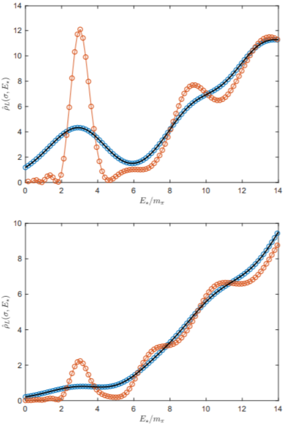
[4]

In the original work [4.], the authors extracted in a synthetic model (system of 3 pions, the kaon K and the ϕ meson) the spectral density $\hat{\rho}_L$, using a Gaussian as a smearing function. To use the Haag-Ruelle formalism the algorithm was changed a little bit using functions with compact support.

$$\mathcal{L}_{int}(x) = \frac{g_\pi}{6}\phi(x)\pi^3(x) + \frac{g_K m_\phi}{2}\phi(x)K^2(x)$$

[4] Martin Hansen, Alessandro Lupo, Nazario Tantalo. On the extraction of spectral densities from lattice correlators. Journal Reference: Phys. Rev. D99, 094508 (2019). arXiv:1903.06476v2

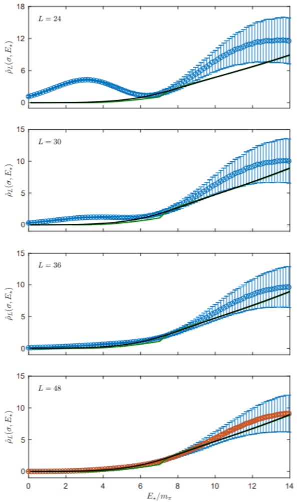
Numerical extraction of ρ



Comparison of the results obtained with the new method (blue points) with the results obtained by using the Backus–Gilbert method (orange points) in the absence of statistical errors. The two plots correspond to the volumes L = 24 and L = 32 with tmax = 30 in both cases. In the case of the new method the results have been obtained by using the Gaussian as target smearing function with $\sigma = 0.1$.

Numerical extraction of ρ

Approach to the infinite–volume limit of the reconstructed smeared spectral densities. The results correspond to $\sigma = 0.1$ and have been obtained by using $b_T(t, E)$ as basis functions with $E_0 = 0$, $T = 2(t_{max} + 1)$ and $t_{max} = 31$. In all plots the green and black curves correspond respectively to the exact infinite–volume unsmeared and smeared spectral densities. The orange band in the last plot corresponds to the statistical uncertainties.



Conclusions and future perspectives

In this Master-thesis work we achieved the following results:

- A non perturbative approach to scattering is necessary in case of hadronic processes $\rightarrow$ it is necessary the link between the S-matrix and the spectral density with the Haag-Ruelle formulation
- Performing a little bit of algebra, we found useful expressions of S-matrix elements, suitable for lattice applications
- Perturbative check and generalization of a pre-existent algorithm.
- Numerical development: extraction of 3-4 points spectral density on 2-d models
- Theoretical development: infinite-volume limit and systematic study of the rate of convergence.

Thank you for your attention!