Analytical prediction for the optical matrix

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We provide an analytical expression and a physical realization of the average ⟨S⟩ of the scattering matrix, called optical S matrix in the nuclear physics jargon. This is done by demonstrating that the large size limit of the scattering matrix, i.e., the fixed point-solution of the recurrence relation of the scattering matrix of a locally periodic system, satisfies the analyticity condition. The obtained optical S matrix, that depends only on the transport properties of a single cell, is used to verify that the Poisson kernel is the distribution of the scattering matrix along the evolution with N to the large size limit. The theoretical distribution shows perfect agreement with numerical results for a chain of delta potentials. A consequence of our findings is the a priori knowledge of the optical S matrix without resort to the experimental data.

INTRODUCTION

Scattering is an outstanding phenomenon of nature concerning waves and particles [1]. It is important in almost all branches of physics since many physical observables, at microscopic and macroscopic scales, are described in terms of scattering properties [2,12]. Among the different mechanisms that occur in complex scattering processes, the direct and equilibrated components can be distinguished. On the one hand, the direct component is a peripheral process which comes from an interaction with a mean field; this smooth part is responsible for a prompt response of the system. On the other hand, the equilibrated response comes from the multiple scattering that gives rise to a delayed response. These two components were introduced firstly in nuclear physics by Feshbach, Porter and Weisskopf, when studying the scattering of a nucleon by an atomic nucleus [13,14]. Secondly, in a seminal paper, Ericson and Mayer-Kuckuk [15] established that “Nuclear-reaction theory is equivalent to the theory of waveguides ...”. Thirdly, the optical model was then applied to problems of scattering through waveguides [3].

In actual experiments, the scattering amplitudes vary with respect to a tuning parameter which could be the energy of incidence in nuclear, many body, and atomic physics [19,15], the Fermi energy or an applied magnetic field in condensed matter physics [19,20], and the frequency in optics [21], microwaves [9,10,22,24], and elastic systems [12,25]. The prompt response is revealed by the average of the measured scattering amplitudes over an interval of the corresponding tuning parameter, the so called optical amplitudes [26]. The delayed response is obtained by subtracting the prompt response to the exact scattering amplitudes. As the tuning parameter varies, the scattering matrix S, formed by the scattering amplitudes, moves on its available space. The way in which it is distributed along this space is determined once the optical matrix ⟨S⟩ is specified, any other information being irrelevant [27].

In an statistical context when the scattering amplitudes not only vary but also fluctuate, with respect to the tuning parameter or sample-to-sample, an ergodic hypothesis is appealed to construct an ensemble of systems, and it is the ensemble average of the scattering amplitudes, at a fixed energy, which reveals the prompt response component [26,28]. In all cases ⟨S⟩ is taken from the experimental or numerical data. The question we want to solve is whether exists the possibility to predict the value of ⟨S⟩ by a procedure that avoids to take the average from the experiment, actual or numeric, at the end.

In this letter the average ⟨S⟩ of the scattering matrix is obtained analytically, through a physical realization,
providing a physical meaning to the large size limit of the scattering matrix expression. We find that it is the evolution with system size which leads to an optical matrix in the large size limit. For locally periodic structures the scattering matrix reaches a fixed point as the number of scatterers goes to infinity [29–31]. This fixed value is of modulus 1 in the gaps, while it is subunitary within the bands. It corresponds to an average with respect to the number of scatterers.

THE MODEL

Let us consider a single port quantum system in one dimension, as shown in fig. 1, it consists of a periodic array with a finite number of identical scattering elements [32–34]. The system with \( N - 1 \) scatterers is described by the \( 1 \times 1 \) scattering matrix \( S_{N-1} \), which is related to the scattering matrix \( S_N \) of a system with \( N \) scatterers. The latter is obtained when another scatterer is added to the system with \( N - 1 \) scatterers. That is, there is a recurrence relation given by [30]

\[
S_N = \frac{r_b' z_b + z_b S_{N-1}^*}{r_b z_b + z_b^* S_{N-1}} S_{N-1}^*,
\]

where \( r_b \) (\( t_b \)) and \( r_b' \) (\( t_b' \)) are the reflection (transmission) amplitudes of an individual scatterer for incidence on the left and right, respectively; \( z_b = t_b e^{i\phi/2} e^{i k (a-b)} \), with \( e^{i\phi/2} = t_b' / t_b \), being \( k \) the incident wave number, \( b \) the width of the scatterer, and \( a \) the lattice constant. Since \( S_N \) depends intrinsically on \( k \), a band structure emerges with respect to \( k \) as \( N \) increases (see fig. 2). The bands and gaps are clearly formed in the crystalline limit \( N \to \infty \), for which eq. (1) has a stable and an unstable fixed point solutions for each value of \( k \); these are [30]

\[
S_\infty(k) = \begin{cases} 
  e^{i\theta_\pm}(k), & k \in \text{gap} \\
  w_\pm(k), & k \in \text{band},
\end{cases}
\]

where

\[
e^{i\theta_\pm}(k) = \pm \sqrt{\frac{|\text{Re } z_b(k)|^2 - |t_b(k)|^2}{r_b(k) z_b(k)} + i \text{Im } z_b(k)},
\]

and

\[
w_\pm(k) = i \sqrt{|t_b(k)|^2 - |\text{Re } z_b(k)|^2 + |\text{Im } z_b(k)|^2}.
\]

The expression for \( S_\infty \) was reported in ref. [30] without any physical interpretation, apart from representing a large size limit value of the scattering matrix. However, we notice that \( S_\infty \) is a complex number of modulus 1 for \( k \) in the gaps, while it is subunitary for \( k \) within the bands, such that it can not represent a scattering matrix because of flux conservation. Here, we assert that \( S_\infty \) represents an average of a scattering matrix. To see this we observe that, from eq. (1),

\[
\lim_{N \to \infty} (S_N^m) = \left( \lim_{N \to \infty} S_N \right)^m = S_\infty^m,
\]

with \( m \) an integer, which resembles the analyticity condition satisfied by the average of the scattering matrix \( S \) [27]. This \( S \)-matrix describes the system that evolves with size. Therefore, we postulate that the limit \( N \to \infty \) corresponds to an averaging procedure,

\[
\langle S^m \rangle = \lim_{N \to \infty} S_N^m = S_\infty^m.
\]

This result is exact and corresponds to an analytical continuation from the gaps to the bands. It is instructive to compare this procedure with the long-time average that leads to the ergodic theorem in statistical mechanics context [35]. There, a sufficiently long time makes that a representative point of a system cover the entire accessible phase space [30]. In a very analogous sense, the \( S \)-matrix visits its available space according to a certain distribution along the evolution with the system size (iteration time). This distribution becomes specified since the analyticity condition, expressed in eq. (5), implies that all of its moments are known \((\langle S^m \rangle = \langle S \rangle^m)\); the resulting distribution can be easily calculated and is given by Poisson’s kernel [3, 26, 27], namely

\[
p_{\langle S \rangle}(S) = \frac{1}{2\pi} \frac{1 - |S|^2}{|S - \langle S \rangle|^2}, \quad \text{with } \langle S \rangle = S_\infty.
\]

Thus, \( p_{\langle S \rangle}(S) \) depends on \( k \) through the reflection and transmission amplitudes of a single scattering element, eqs. (3) and (4).

ANALYTICAL PREDICTION VS NUMERICS

Here, the main contribution is the prediction (1), together with the condition (5), which implies the Poisson kernel distribution (7). Although the prediction for \( \langle S \rangle \) is completely general, it is tested for a specific chain of potentials. We verify that the histogram for the phase of \( S \), obtained from the numerical data of \( N \) values at fixed \( k \) via the recurrence relation (1), fits the theoretical distribution (7) with \( \langle S \rangle \) calculated from eq. (1). Also, we compare these results with Poisson’s kernel in which \( \langle S \rangle \) is calculated from the numerical data. The quantum chain of delta potentials, as the one shown in the lower part of fig. 1, will be used as example [30]. The energy of the particle will be smaller than the height \( V_0 \) of the step potential, on the left side of the chain, to get a \( 1 \times 1 \) scattering matrix. In this case \( r_b = r_b^* = -u/(u - 2ik) \) and \( t_b = t_b^* = -2ik/(u - 2ik) \), with \( u \) the intensity of the delta potential in the same units as the wave number. The initial condition \( S_0 = e^{i\pi} \), which corresponds to \( V_0 \to \infty \), will be taken.
FIG. 2. Phase of the scattering matrix as a function of $ka$. In (a) we plot the last 30 of 1000 iterations of the recurrence relation and the analytical expression for the stable solution of eq. (2). We observe that the stable solution is indistinguishable from the numerical result in the gaps, while it gives the maximum in the bands (light line). In (b) we show the evolution of the phase from $N = 1$ up to $N=30$.

In fig. 2 the phase of the scattering matrix is plotted for $u_A = 10$ as a function of $ka$ (dimensionless quantities are used). In fig. 2 (a) the last 30 of 1000 iterations are plotted, as well as the fixed point solution (we show only the stable solution) which is highlighted in the bands but it is indistinguishable from the numerical result within the gaps. In fig. 2 (b) the first 30 iterations show the distribution of points around a maximum value given by the fixed point solution.

The numerical distributions of $N = 10^4$ scattering systems are shown as histograms in fig. 3 for several values of $k$. In fig. 3 (a) we observe that, for $k$ in the gap, the distribution is just a delta function at the stable fixed point solution. This is due to the fact that the fixed point solution is exponentially reached in the limit $N \to \infty$ [30] and there is not enough “time” to $S$ to be distributed on the available space. Something similar happens for the unstable fixed point solution in which the phase remains there always and it is not distributed in the whole interval. In contradistinction, for $k$ inside but close to the border of the band, and inside the band, panels (b), (c) and (d) of fig. 3, respectively, show that the phase of $S$ is distributed in the complete space between 0 and $2\pi$. However, at the transition the distribution is narrower than the distribution for $k$ close to the center of the band: closer to the transition, narrower the distribution is. It is explained from the fact that inside the band $S$ has enough “time” to visit the whole space but this “time” is reduced as $k$ approaches the transition. There, the fixed point solution is reached as a power law [50]. In all of the cases shown, the histograms have an excellent agreement with the Poisson kernel [7] for $\langle S \rangle$ calculated from eqs. (2) and (6), as well as when it is calculated from the numerical data. This excellent agreement shows that $S_\infty$ certainly is the optical matrix $\langle S \rangle$.

CONCLUSIONS

In conclusion, an analytical expression for the average of the scattering matrix, known as the optical matrix in the nuclear physics jargon, was provided. This was done by demonstrating that the fixed point solution of the recurrence relation of the scattering matrix, of a locally periodic system, where the recurrence time is just the number $N$ of scatterers, satisfies the analyticity condition. When $N \to \infty$ a perfect crystal, with bands and gaps, is obtained. This limit is equivalent to an average procedure and the fixed-point solution of the scattering matrix corresponds to the optical matrix. This was verified by using the fixed point solution in the expression of Poisson’s kernel. The theoretical distribution fits perfectly the histogram obtained from numerical iterations for a chain of delta potentials. The same is valid when the optical matrix is obtained from the numerical average of the scattering matrix over all different configurations of $N$. It is important to remark that, in this way, the large size limit of the scattering matrix can be interpreted as the optical $S$ matrix.

We proved our assertion for a single port one-dimensional problem, without loss of generality, although the extension to higher dimensions is direct. Although our assertion was proved for a single port one-dimensional
problem, the extension to higher dimensions is direct since (i) it has been shown that the large size limit value of the scattering matrix in a two port systems has similar properties [31] and (ii) it is well known the Poisson kernel expression for higher dimensions [27]. Other wave phenomena, like dissipation, have drastic effects on the scattering properties are left for the next future.

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