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Study of a quantum scattering process by means of entropic measures

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ABSTRACT

In this Letter, a scattering process of quantum particles through a potential barrier is considered. The statistical complexity and the Fisher–Shannon information are calculated for this problem. The behaviour of these entropy-information measures as a function of the energy of the incident particles is compared with the behaviour of a physical magnitude, the reflection coefficient in the barrier. We find that these statistical magnitudes present their minimum values in the same situations in which the reflection coefficient is null. These are the situations where the total transmission through the barrier is achieved, *the transparency points*, a typical phenomenon due to the quantum nature of the system.

The study of the crossing of potential barriers by wave functions is useful for the understanding of many interesting quantum phenomena, such as tunneling [1], interferences [2], resonances [3], electron transport [4], etc., and presents some similarity with other wave phenomena such as the transmission of light in materials [5].

In this Letter, we take the most tractable case, the plain square barrier, that is a standard set-up for many theoretical purposes [6] and can be useful for our present goal, namely, to check the behaviour of different statistical magnitudes in the scattering process of quantum particles.

The calculation of information theory measures in quantum bound states has been performed for different systems in the last years [7–14]. These statistical quantifiers have revealed a connection with physical measures, such as the ionization potential and the static dipole polarizability in atomic physics [15,16]. Other relevant properties concerning the bound states of atoms and nuclei have been put in evidence when computing these indicators on these many-body systems. For instance, the extremal values of these measures on the closure of shells [17,18] and the trace of magic numbers [19,20] are some of these properties.

The evaluation of these magnitudes in a quantum system requires the knowledge of the probability density as the basic ingredient. For bound states, this is directly known in some cases such as the H-atom [8] or numerically derived in other cases from a Hartree–Fock scheme [21,22]. For no bound states, we proceed in this Letter to show how to perform this calculation. We address this objective in the particular case of the scattering process of quantum particles through a potential barrier. The simplest obstacles which can be studied are the square barrier and the square well, two physical set-ups that can receive an equivalent mathematical treatment. In our case, the phenomenon of reflection (or transmission) of a wave function through a rectangular potential barrier in a one-dimensional set-up is considered [6]. This standard system presents three different regions depending on the value of the potential $V(x)$,

$$V(x) = \begin{cases} 0, & x \leqslant 0 \text{ (Region I)}, \\ V_0, & 0 < x < L \text{ (Region II)}, \\ 0, & x \geqslant L \text{ (Region III)}, \end{cases} \tag{1}$$

with L and V_0 the width and height of the barrier, respectively.

When the free particle of mass m encounters the barrier from the left for an energy $E > V_0$, the solution $\phi(x)$ of the time-independent Schrödinger equation for the potential (1) can be written as

$$\phi(x) = \begin{cases} \phi_I(x) = A_1 e^{ik_1 x} + A'_1 e^{-ik_1 x}, \\ \phi_{II}(x) = A_2 e^{ik_2 x} + A'_2 e^{-ik_2 x}, \\ \phi_{III}(x) = A_3 e^{ik_1 x}, \end{cases} \tag{2}$$

where there is no reflected wave ($e^{-k_1 x}$ term) in the Region III. The expressions for the wave numbers are: $k_1 = \sqrt{2mE/\hbar^2}$ and $k_2 = \sqrt{2m(E - V_0)/\hbar^2}$, with $\hbar$ the Planck's constant. Observe that when the particle comes in through the barrier with an energy $0 \leqslant E \leqslant V_0$, the wave number k_2 becomes imaginary, then $\phi_{II}(x) = A_2 e^{\rho_2 x} + A'_2 e^{-\rho_2 x}$, with $\rho_2 = \sqrt{2m(V_0 - E)/\hbar^2}$. The five

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amplitudes $(A_1, A_2, A_3, A_1', A_2')$ are complex numbers determined, up to a global phase factor, by the normalization condition and the boundary constraints, namely the continuity of the wave function and its derivative at $x = 0$ and $x = L$.

The scattering region (Region II) provokes a partial reflection of the incident wave. The reflection coefficient R gives account of the proportion of the incoming flux that is reflected by the barrier. The expression for R is:

$$R = \frac{Flux_{reflected}}{Flux_{incident}} = \frac{|A_1'|^2}{|A_1|^2}. \quad (3)$$

In this process, there are no sources or sinks of flux, then the transmission coefficient T is given by $T = 1 - R$.

It is straightforward to see that depending on the energy of the incident particles there are two different behaviours in the scattering process, let us say the cases $0 \leqslant E \leqslant V_0$ and $E > V_0$. If we write the energy of the particles as $E = pV_0$ with p a non-dimensional parameter, then the cases to study are: $0 \leqslant p \leqslant 1$ and $p > 1$.

The reflection coefficient for $p > 1$ yields:

$$R = \frac{(k_1^2 - k_2^2)^2 \sin^2(k_2 L)}{4k_1^2 k_2^2 + (k_1^2 - k_2^2)^2 \sin^2(k_2 L)} = \frac{\sin^2(k_2 L)}{4p\,(p-1) + \sin^2(k_2 L)}, \quad (4)$$

and for $0 \leqslant p \leqslant 1$ is:

$$R = \frac{(k_1^2 + \rho_2^2)^2 \sinh^2(\rho_2 L)}{4k_1^2 \rho_2^2 + (k_1^2 + \rho_2^2)^2 \sinh^2(\rho_2 L)} = \frac{\sinh^2(\rho_2 L)}{4p\,(1-p) + \sinh^2(\rho_2 L)}. \quad (5)$$

In order to compute the reflection coefficient R, it is necessary to give some concrete values to the size of the barrier and the mass of the particles. For the plots presented in Figs. 1–4, we have taken $V_0 = 1$ eV, $L = \lambda L_0$ with $L_0 = 10$ Å and λ a positive real constant, and $m = 0.511$ MeV the electron mass. For these values, we find that

$$k_2 L = 5.123\,\lambda\,\sqrt{p-1}, \quad (6)$$

and

$$\rho_2 L = 5.123\,\lambda\,\sqrt{1-p}. \quad (7)$$

We also proceed to calculate two statistical magnitudes for this problem, the statistical complexity and the Fisher–Shannon entropy. These magnitudes are the result of a global calculation done on the probability density $\sigma(x)$ given by $\sigma(x) = |\phi(x)|^2$, taking into account that the interval of integration must be adequate to impose the normalization condition in the wave function. Particularly, this interval of integration is taken to be $[-a, 0]$, $[0, L]$ and $[L, L + a]$, with $a = \pi/k_1$, for Regions I, II and III, respectively.

The statistical complexity C [23,24], the so-called LMC complexity, is defined as

$$C = H \cdot D, \quad (8)$$

where H is a function of the Shannon entropy of the system and D gives account of the sharpness of its spatial configuration. Here, H is calculated according to the simple exponential Shannon entropy S [24–26], that has the form,

$$H = e^S, \quad (9)$$

with

$$S = -\int \sigma(x)\,\log \sigma(x)\,dx. \quad (10)$$

For the disequilibrium D, we take some kind of distance to the equiprobability distribution [23,24], that is,

$$D = \int \sigma^2(x)\,dx. \quad (11)$$

The Fisher–Shannon information P [27–29] is defined as

$$P = J \cdot I, \quad (12)$$

where the first factor is a version of the exponential Shannon entropy [26],

$$J = \frac{1}{2\pi e} e^{2S}, \quad (13)$$

with the constant 2 in the exponential selected to have a non-dimensional P. The second factor

$$I = \int \frac{[d\sigma(x)/dx]^2}{\sigma(x)}\,dx, \quad (14)$$

is the so-called Fisher information measure [30], that quantifies the roughness of the probability density.

The reflection coefficient, R, and the statistical complexity, C, for the low energetic particles, $0 < p < 1$, in Region I are plotted in Fig. 1. For small p, there is no penetration of the flow and the particles are reflected in the barrier, that is, $R = 1$. The interference between the incident and the reflected waves generates standing waves in this Region I, given that both of them have the same wave number and the same amplitudes. The complexity of any standing wave is $C = 3/e \simeq 1.1036$. This value also corresponds to the complexity calculated for the eigenstates of the infinite square well [31]. When the energy of the particles approaches the height of the barrier, i.e. $p \lesssim 1$, the tunnel effect becomes perceptible and some transmission through the barrier takes place, then $R \lesssim 1$. It can be clearly seen in Fig. 1(a) better than in Fig. 1(b) due to the different widths of the barrier, $\lambda = 2$ and $\lambda = 5$, respectively. Despite the tunnel effect, the most of the flow is reflected in the barrier and the standing waves are maintained in the Region I, then C does not register any change.

In Fig. 2, the behaviour of R and C for particles with higher energies than the height of the barrier, i.e. $p > 1$, is shown in Region I. First, the continuity of R and C for $p = 1$ is observed with respect to the values taken in Fig. 1. Second, the transmission of particles becomes more important as their energy increases. In the limit $p \gg 1$, the totality of the flow goes through the barrier, then there is no reflected wave and R decays to zero with a power law, p^{-2}, as it can be obtained from Eq. (4). Third, the quantum nature of the problem appears in the oscillatory behaviour of the reflection coefficient. When the condition of standing wave in the barrier is reached, that is, $k_2 L = n\pi$ with $n = 1, 2, \ldots$, the barrier becomes transparent and the totality of the flow is transmitted, then $R = 0$. The values of the energy that fulfil this condition are given by the following series of p values:

$$p = 1 + \left(\frac{\pi}{5.123\,\lambda}\right)^2 n^2, \quad n = 1, 2, 3 \ldots. \quad (15)$$

Observe that the density of zeros for R increases with λ, the width of the barrier, as it can be seen in Figs. 2(a) and 2(b), where $\lambda = 2$ and $\lambda = 5$, respectively. Finally, observe that C also presents an oscillatory behaviour with an asymptotic decay to $C = 1$ when $p \gg 1$. Remark that C takes its minimum value $C = 1$ just on the transparency points p, given by the series of values (15), where the particles, similarly to the case $p \gg 1$, are plane waves in the Region I and then they generate a constant density on this region, which is the situation of minimum complexity. In between