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LONG TIME BEHAVIOR OF CORRELATION FUNCTIONS: CONNECTIONS BETWEEN SYSTEM AND MEASURED QUANTITIES

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ABSTRACT. In the present paper an approach concerning the formalism of time dependent Pair Correlation Functions (PCF), which characterize the time-space properties of material systems and their Fourier Transforms (FT) is presented. In particular, the effects of the system-probe interaction are dealt by taking into account the coupling between the system properties, through the PCF, and the instrument response function, through its resolution function. Such an approach shows the effects of the instrumental resolution function on the time dependent PCF and on its FT. It emerges that the system dynamics that occurs on a time scale longer than the instrumental energy resolution, is entirely summed up in the elastic contribution whereas the system dynamics on a time scale shorter than the instrumental energy resolution is weighted by the resolution function. As a consequence, by changing the instrumental resolution one can register a crossover between a condition dominated by the elastic contribution to a condition dominated by the quasi-elastic contribution; this occurs when the system relaxation time matches the instrumental resolution time. This procedure reveals to be useful for the analysis of elastic and quasi-elastic signals.

1. Introduction

Molecular dynamics (MD) and spectroscopic techniques furnish powerful investigation tools for obtaining information on the space-time correlations in condensed matter systems. As a rule, with MD one considers a set of n_{tot} particles, chooses an intermolecular potential, fixes boundary and initial conditions and then solves the $6n_{tot}$ coupled equations of motion. From the equation solutions one can calculate equilibrium as well as time dependent quantities associated to the system. On the other hand, by spectroscopic techniques one deals with a probe, usually prepared in a well-known initial state, able to properly interact with the system; due to the interaction, the probe state changes and this change reflects some of the system properties. The result generally appears in the form of a quantity which can be connected with a well-defined Pair Correlation Function (PCF). More in detail, let us take into account a material system, M, composed by n_{tot} (typically $n_{tot} \simeq 10^3$) particles i , at the thermal equilibrium, which is characterized by an Hamiltonian H_M whose eigenvalues and eigenstates are labelled E'_m and $|m' >$ (Volino 1978). Let P be a probe characterized by an Hamiltonian H_P whose eigenvalues and eigenstates are labelled E_m and $|m >$ and which is able to couple with M, the coupling being characterized by an Hamiltonian H_C. Since M is at thermal equilibrium at a temperature T, it can be in any state $|m' >$ with the probability p'_m given by the Boltzmann law $p'_m = \frac{1}{Z_M} exp(-\beta E'_m)$ with $z_M = \sum'_m(-\beta E'_m)$ and $\beta = \frac{1}{k_B T}$, where $k_B T$ is the Boltzmann constant. Due to the probe-system coupling, the state of P can change with time from an initial state $|m >$ to a final state $|n >$. In the linear approximation (i.e. if H_C is small compared to H_P and H_M), and in the long time range, it is possible to characterize this change by a probability per unit time, W_{nm}, which can be connected to the Fourier Transform (FT) of a well-defined PCF. This W_{nm}-PCF relationship is clearly dependent on the type and details of the specific experiment to be performed and, hence, no general formula can be given. In the following the effects of the system-probe interaction will be dealt in order to show the effects of the instrumental resolution function on the time dependent PCF and on its FTs. The approach, which is developed also in terms of matrices, shows the connection between the PCF long time limit, its FT and the instrumental time resolution.

2. 2D FT as compound operator of two 1D FT

A common definition of FT for two dimensions functions is:

$$F(u,v) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x,y) e^{-2\pi i(ux+vy) dxdy} \tag{1}$$

To which the following inverse formula corresponds:

$$f(x,y) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} F(u,v) e^{2\pi i(ux+vy) dudv} \tag{2}$$

In general, FT is a complex function of real variables; as such, for practical purposes, the transform can be expressed in terms of its magnitude and phase. It is important to stress that the 2D FT can be implemented as a sequence of 1D FT operations performed independently along the two function variables:

$$\begin{aligned} F(u,v) &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x,y) e^{-2\pi i(ux+vy) dxdy} \\ &= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x,y) e^{-2\pi iux} e^{-2\pi ivy} dxdy \\ &= \int_{-\infty}^{+\infty} f(x,y) e^{-2\pi iux} dx \int_{-\infty}^{+\infty} f(x,y) e^{-2\pi ivy} dy \\ &= \int_{-\infty}^{+\infty} F(u,v) e^{-2\pi ivy} dy = F(u,v) \end{aligned} \tag{3}$$

Figure 1 summarizes the 2D dimensional FT as a sequence of two 1D FT operations performed independently along the two variables.

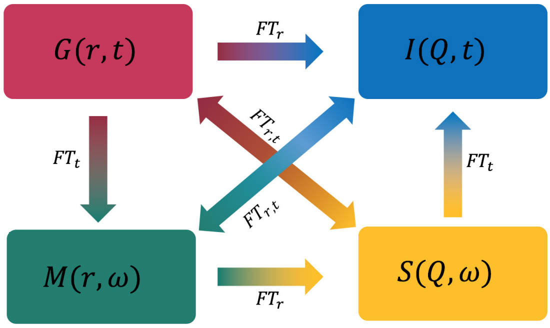

FIGURE 1. 2D dimensional FT as a sequence of two 1D FT operations performed independently along the two variables.

3. Ideal case of separable functions

In the ideal case in which the function $f(x,y)$can be written as $f(x,y) = h(x)k(y)$, i.e. in the case in which $f(x,y)$is a separable function, its FT is the product of the FTs of the two functions $h(x)$,$k(y)$:

$$
\begin{aligned}
F(u,v) &= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)e^{-2\pi i(ux+vy)dxdy} \\
&= \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} h(x)k(y)e^{-2\pi iux}e^{-2\pi ivy}dxdy \\
&= \int_{-\infty}^{+\infty} h(x)e^{-2\pi iux}dx \int_{-\infty}^{+\infty} k(y)e^{-2\pi ivy}dy \\
&= H(u)K(v)
\end{aligned}
\tag{4}
$$

$$
f(x,y) = h(x)k(y) \Rightarrow F(u,v) = H(u)K(v) \tag{5}
$$

An example of separable function is furnished by the two dimensional Gaussian:

$$
f(x,y) = e^{-x^2-y^2} \tag{6}
$$

As in the case of 1D Gaussian function, the FT of a 2D Gaussian is a 2D Gaussian function (Cochran 1967; Lim 1990; Alleyne and Cawley 1991), as reported in Figure 2.

Experimental examples of separable functions, which are Gaussians, are furnished by instrumental resolution functions.

4. Time dependent pair correlation functions

Considering now the particle system M, following Van Hove (Van Hove 1954), one can introduce the system time dependent pair correlation function $G(r,t)$, defined as:

$$
G(r,t) = \frac{1}{n_{tot}}\langle\sum_{i,j}^{N}\int d\mathbf{r}'\cdot\delta(\mathbf{r}+\mathbf{r}_i(0)-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}_j(t))\rangle \tag{7}
$$

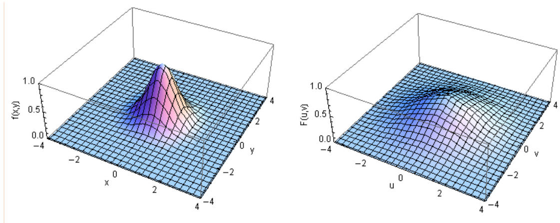

FIGURE 2. Two dimensional Gaussian function$f(x,y) = e^{-x^2}e^{-y^2}$ (on the left) with its Fourier Transform $F(u,v) = \frac{e^{\frac{u^2}{4}\frac{v^2}{4}}}{2}$ (on the right).

where **r**' refers to an integration variable and the angle brackets < > denote an ensemble average. $G(r,t)$ can be interpreted as the probability to find a particle j at time t at the place r if this or another particle i was at time $t = 0$ at the origin $r = 0$, so describing how the correlation between the particle positions evolves with time. The one dimensional spatial Fourier Transform, FT_r, of the time dependent pair correlation function is called the intermediate scattering function $I(Q,t)$ (Van Hove 1954):

$$FT_r[G(r,t)] = I(Q,t) \tag{8}$$

By introducing the two dimensional space-time Fourier Transform, $FT_{r,t}$, one can introduce the system scattering law $S(Q,\omega)$[5]:

$$FT_r[G(r,t)] = S(Q,\omega) \tag{9}$$

$$S(Q,\omega) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} G(r,t)e^{-2\pi i(Qr+\omega t})drdt \tag{10}$$

In the case of systems which can be regarded as composed of distinguishable particles the $G(r,t)$ function splits in two contributions:

$$G(r,t) = G_s(r,t) + G_d(r,t) \tag{11}$$

$G_s(r,t)$, where the subscript s stands for "self", describes the correlation between positions of one and the same particles at different times, while $G_d(r,t)$, where the subscript d stands for "distinct", refers to pairs of distinct particles (H. Freed 1978; Magazù 2000; Branca *et al.* 2003b; Hopkins *et al.* 2010). More precisely, they are defined as follows:

$$G_s(r,t) = \frac{1}{n_{tot}}\langle\sum_{j=1}^{n_{tot}}\int d\mathbf{r}'\cdot\delta(\mathbf{r}+\mathbf{r}_j(0)-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}_j(t))\rangle \tag{12}$$

$$G_d(r,t) = \frac{1}{n_{tot}}\langle\sum_{j\neq i=1}^{n_{tot}}\int d\mathbf{r}'\cdot\delta(\mathbf{r}+\mathbf{r}_i(0)-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}_j(t))\rangle \tag{13}$$

In other terms, $G_s(r,t)$ can be interpreted as the probability to find one particle at time t at place r if the same particle was at time $t = 0$ at $r = 0$. $G_d(r,t)$ can be interpreted as the probability to find at time t at place r one particle distinct from the one that was at the origin at time . More precisely, for short times, the self correlation function $G_s(r,t)$ approximates to a δ-function, while the distinct correlation function $G_d(r,t)$ is approximately the radial distribution function (Egelstaff 1992; Magazù 1996; Magazù *et al.* 2004b, 2011b).

For large times, as $t \longrightarrow \infty G_d(r,\infty) \approx \rho$, which is the density of system, given by $\frac{n_{tot}}{V}$, where is the volume. Similarly, for the $G_s(r,\infty) = 1/V$, that tends to zero when V tends to ∞ . In other, words, $G_(r,t) \longrightarrow 0$ and $G_d(r,t) \longrightarrow \rho$. The qualitative behavior of $G_s(r,t)$ and $G_d(r,t)$ are reported in Figure 3.

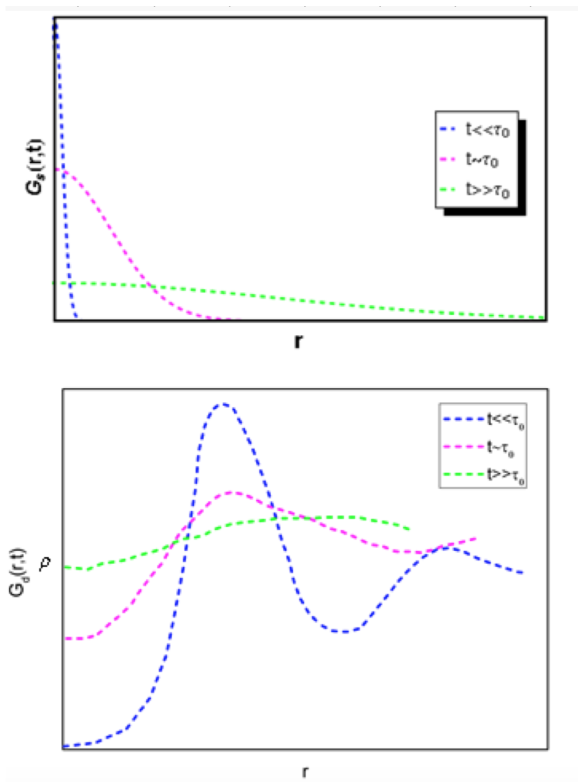

FIGURE 3. Qualitative behavior of $G_s(r,t)$, i.e. the self term, and $G_d(r,t)$, i.e. the distinct term, for several value of t. In the top (a) $G_s(r,t)$ is shown, in the bottom (b) $G_d(r,t)$; τ is the system relaxation time.

It results:

$$FT_r[G_s(r,t)] = I_s(Q,t) \tag{14}$$

$$FT_r[G_d(r,t)] = I_d(Q,t) \tag{15}$$

The one dimensional time FT, FT_t of the intermediate scattering function is the scattering function $S(Q,\omega)$ (Middendorf *et al.* 2000; Magazù *et al.* 2001a):

$$FT_t[I(Q,t)] = S(Q,\omega) \tag{16}$$

It results:

$$FT_t[I_s(Q,t)] = S_s(Q,\omega) \tag{17}$$

$$FT_t[I_d(Q,t)] = S_d(Q,\omega) \tag{18}$$

By introducing the two dimensional space-time FT, $FT_{r,t}$, one can write:

$$FT_{r,t}[G(r,t)] = S(Q,\omega) \tag{19}$$

The quantity:

$$M(r,\omega) = FT_t[G(r,t)] = FT_r[S(Q,\omega)] = FT_{r,t}[I(Q,t)] \tag{20}$$

is called *dynamic correlation function*.

From the experimental point of view, as an example, one can take into account the case of neutron scattering, indicating with b_α and b_β the scattering lengths of atom α and β respectively, $|\bar{b}|^2 = \langle b^*_\alpha b_\beta \rangle$, $\overline{|b|^2} = \langle b^*_\alpha b_\alpha \rangle$, $\sigma_d = 4\pi|\bar{b}|^2$ and $\sigma_s = 4\pi\left(|\bar{b}|^2 - \overline{|b|^2}\right)$ where σ_d takes into account interference effects among waves produced by the scattering of a single neutron from all the system nuclei whereas σ_s refers to single particle properties (Branca *et al.* 1999a,b); in such a case the neutron scattering double differential cross section, indicating with k_0 and k_1 the incoming and outcoming neutron wavevectors, can be written as:

$$\begin{aligned}
\frac{d^2\sigma}{d\Omega d\omega} &= \frac{k_1}{k_0}\frac{1}{2\pi}\int_{-\infty}^{+\infty} dt e^{-i\omega t}\frac{1}{N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}\langle b^*_\alpha b_\beta e^{-i\mathbf{Q}\cdot\mathbf{R}_\alpha(0)} e^{-i\mathbf{Q}\cdot\mathbf{R}_\beta(t)}\rangle \\
&= \frac{k_1}{k_0}\frac{1}{2\pi}\int_{-\infty}^{+\infty} dt e^{-i\omega t}\frac{1}{N}\left[|\bar{b}|^2\sum_{\alpha}\sum_{\alpha\neq\beta}\langle e^{-i\mathbf{Q}\cdot\mathbf{R}_\alpha(0)} e^{-i\mathbf{Q}\cdot\mathbf{R}_\beta(t)}\rangle + \overline{|b|^2}\langle e^{-i\mathbf{Q}\cdot\mathbf{R}_\alpha(0)} e^{-i\mathbf{Q}\cdot\mathbf{R}_\alpha(t)}\rangle\right] \\
&= \frac{k_1}{k_0}|\bar{b}|^2 S_d(Q,\omega) + \frac{k_1}{k_0}\overline{|b|^2} S_s(Q,\omega) + \frac{k_1}{k_0}\left(|\bar{b}|^2 - \overline{|b|^2}\right) S_inc(Q,\omega) \\
&= \frac{k_1}{k_0}|\bar{b}|^2 S_d(Q,\omega) + \frac{k_1}{k_0}\left(|\bar{b}|^2 - \overline{|b|^2}\right) S_s(Q,\omega) \\
&= \frac{k_1}{k_0}\frac{\sigma_d}{4\pi} S_d(Q,\omega) + \frac{k_1}{k_0}\frac{\sigma_s}{4\pi} S_s(Q,\omega) \\
&= \frac{k_1}{k_0}\left[\frac{\sigma_d}{4\pi} S_d(Q,\omega) + \frac{\sigma_s}{4\pi} S_s(Q,\omega)\right]
\end{aligned} \tag{21}$$

In the case of a high percentage of hydrogen atoms in the investigated system only this latter contribution will be relevant (Branca *et al.* 2002b; Migliardo *et al.* 2013, 2014):

$$\frac{d^2\sigma}{d\Omega d\omega} \cong \frac{k_1}{k_0}\left[\frac{\sigma_s}{4\pi} S_s(Q,\omega)\right] \tag{22}$$

Figure 4 summarizes the space and time FT relations existing between the introduced functions, i.e. $G(r,t), I(Q,t), S(Q,\omega)$ and $M(r,\omega)$:

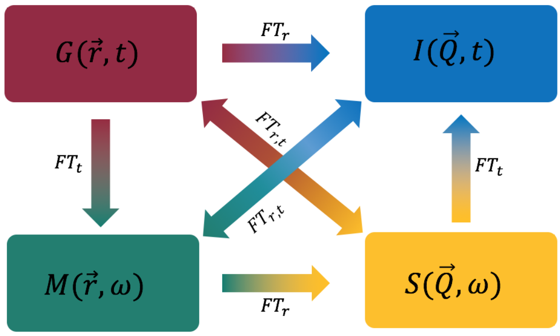

FIGURE 4. Sketch of the one and two dimensional space-time Fourier transform connections among system quantities.

Taking into account the properties of the two dimensional FT we can assume that $G(r,t) = G(r_i,t_j)$ (see 5) and hence we can apply the FT$_r$ to each $G(r_i,t_j)$ raw, keeping constant t_j and the FT$_t$ to each $G(r_i,t_j)$ column, keeping constant r$_i$.

G(1,1)	G(1,2)	...	G(i,j)	...	G(1,n-1)	G(1,n)
G(2,1)						
...						
G(i,1)						
...						
G(m-1,1)						
G(m,1)						

FIGURE 5. $G(r_i,t_j)$ $m \times n$ array.

Therefore, the two dimensional FT is achieved by first transforming in respect to each row, i.e. by replacing each row with its FT transformed row, and then transforming each column, replacing each column with its FT column. Figure 6 shows the FT operations in terms of functions and matrix elements.

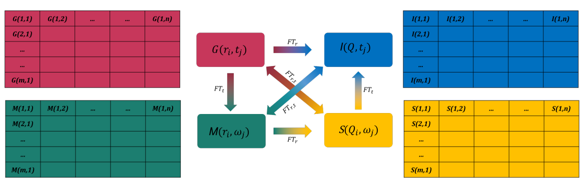

FIGURE 6. Sketch of the one and two dimensional space and time Fourier transform connections among system quantities in terms of functions (inner rectangles) and of the corresponding arrays (outer rectangles).

5. Windowed Fourier Transform

Let us introduce now the Windowed Fourier Transform (WFT) which is defined as (Huang *et al.* 2010; Fernandez *et al.* 2011; Chen *et al.* 2013; Johnson 2013):

$$W(u,v,\xi,\eta) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)g(x-u,y-v)e^{-[2\pi i(\xi x+\eta y)]}dxdy \tag{23}$$

Where $f(x,y)$ is a 2D signal, and $g(x,y)$ is a sliding window function. In other terms, one multiplies the $f(x,y)$ 2D signal by a moving window $g(x-u,y-v)$ and then one computes the FT of the windowed signal $f(x,y)g(x-u,y-v)$. The WFT can be also viewed as a measure of the "affinity" between the original 2D signal $f(x,y)$ and the time-shifted and frequency-modulated window function $g(x,y)$ (Harris 1978; Rahmi Canal 2010). In such a way, the signal $f(x,y)$ is chopped up into segments and each segment is analyzed for its frequency content separately. Different types of window functions have been developed in literature, each of them being specifically tailored for a particular application (Gabor 1947; Wang and Da 2012). As mentioned above, one the most common window profiles for the instrumental resolution functions, is constituted by a Gaussian:

$$g(x,y) = \frac{1}{\sqrt{2\pi\sigma_x\sigma_y}}e^{-\left(\frac{x^2}{\sigma_x^2}+\frac{y^2}{\sigma_y^2}\right)} \tag{24}$$

where σ_x and σ_y are the standard deviations of the Gaussian function in x and y directions, respectively. The Gaussian based WFT is called Gabor transform and was firstly proposed by Dennis Gabor in 1946 (Gabor 1947; Cohen 1966, 1989).

6. Measured correlation functions

Let us take into account now that the previously introduced functions, i.e. $G(r,t)$, $I(Q,t)$, $S(Q,\omega)$ and $M(r,\omega)$ make reference to the system properties to be investigated; however these functions do not represent the quantities accessible by means of measurement processes. In particular introducing the instrumental resolution function $R(r,t)$, we have that, for example, the "measured" scattering law $S_R(Q,\omega)$ is given by the 2D convolution product of the scattering law $S(Q,\omega)$and instrumental law $R(Q,\omega)$:

$$S_R(Q,\omega) = S(Q,\omega)\otimes_r\otimes_t R(Q,\omega) \tag{25}$$

Where now the double notation of $\otimes_r\otimes_t$ is used both to emphasize that this is a 2D convolution and to better distinguish it from a 1D convolution; more precisely $\otimes_r$ denotes the space product convolution and $\otimes_t$ denotes the time product convolution. Since the FT of the convolution of two functions is the product of their individual FT, by using the notation that the subscript R refers to "measured" quantities, it results (Rahman *et al.* 1962; Sakai and Arbe 2009; Magazù *et al.* 2012b; Magazù *et al.* 2013a; Magazù and Migliardo 2013; Magazù *et al.* 2016, 2018):

$$FT[S_R(Q,\omega)] = G_R(r,t) \tag{26}$$

On the other hand, one has:

$$FT[G_R(r,t)] = S_R(Q,\omega) \tag{27}$$

In particular, in the general case in which the introduced function is not separable it results:

$$\begin{aligned} S_R(Q,\omega) &= S(Q,\omega) \otimes_r \otimes_t R(Q,\omega) \\ FT_{r,t}[S_R(Q,\omega)] &= FT_{r,t}[S(Q,\omega)] \cdot FT_{r,t}[R(Q,\omega)] \\ FT_t[FT_{r,t}[S_R(Q,\omega)]] &= Ft_t[FT_{r,t}[S(Q,\omega)]] \cdot FT_t[FT_{r,t}[R(Q,\omega)]] \\ FT_t[M_R(Q,\omega)] &= FT_t[M(r,\omega)] \cdot FT_t[R(r,\omega)] \\ G_R(r,t) &= G(r,t) \cdot R(r,t) \end{aligned} \tag{28}$$

On the other hand, one has:

$$\begin{aligned} G_R(r,t) &= G(r,t) \cdot R(r,ta) \\ FT_{r,t}[G_R(r,t)] &= FT_{r,t}[G(r,t)] \otimes_r \otimes_t FT_{r,t}[R(r,t)] \\ FT_r[FT_t[G_R(R,T)]] &= FT_r[FT_t[G(r,t]] \otimes_r \otimes_t FT_r[FT_t[R(r,t)]] \\ FT_r[M_R(r,\omega)] &= FT_r[M(r,\omega)] \otimes_r \otimes_t FT_r[R(r,\omega)] \\ S_R(r,\omega) &= S(Q,\omega) \otimes_r \otimes_t R(Q,\omega) \end{aligned} \tag{29}$$

Figure 7 summarizes the space and time FT connections existing among the "measured" $G_R(r,t)$, $S_R(Q,\omega)$, $I(Q,t)$ and $M_R(r,\omega)$.

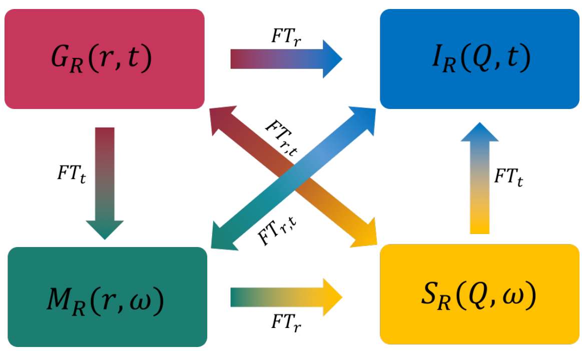

FIGURE 7. Sketch of the one and two dimensional space and time FT connections among the "measured" quantities: $G_R(r,t)$, $S_R(Q,\omega)$, $I(Q,t)$ and $M_R(r,\omega)$.

So, from a formal point of view, the convolution of the two function $S(Q,\omega)$ and $R(Q,\omega)$ produces a third function $S_R(Q,\omega)$ which can be viewed as modified version of the original function. When one is interested only on the ω behavior, assuming that the instrumental function $R(Q,\omega)$ is symmetric in ω then the convolution coincides with the cross-correlation between $S(Q,\omega)$ and $R(Q,\omega)$ (Magazù *et al.* 2008b, 2009, 2010a; Magazù *et al.* 2010b; Magazù *et al.* 2011a, 2012a, 2013b).

By using the convolution theorem one gets:

$$\begin{aligned} S_R(Q,\omega) &= S(Q,\omega) \otimes_t R(Q,\omega) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} I(Q,t) \cdot R(Q,t) e^{-i\omega t} dt \end{aligned} \tag{30}$$

If $I(Q,t)$ is an even function of t, as for example it occurs when one is dealing with incoherent scattering, and $R(Q,t)$ is even too, then also their product is an even function (Magazù *et al.* 2005, 2006a,c, 2007; Magazù *et al.* 2008a; Magazù *et al.* 2008c,d). This circumstance allows one to consider the cosine Fourier transform, i.e.:

$$\begin{aligned} S_R(Q,\omega) &= S(Q,\omega) \otimes_t R(Q,\omega) \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} I(Q,t) \cdot R(Q,t) cos(\omega t) dt \\ &= FT_{resolution \quad windowed}[I(Q,t)] = Gabor \quad transform \end{aligned} \tag{31}$$

In other terms, the resolution windowed FT coincides with the Gabor transform. In the ideal case of a purely elastic scattering, the resolution function is a delta function in the ω-space and, hence, a constant in the t-space,

$$R(Q,\omega) = \delta(\omega) \equiv R(Q,t) = const. \tag{32}$$

in such a case one obtains from Eq. (30) that the measured scattering law is proportional to the scattering law (see 8):

$$\begin{aligned} S_R(Q,\omega) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} I(Q,t) \cdot R(Q,t) cos(\omega t) dt \\ &= \frac{const.}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} I(Q,t) cos(\omega t) dt = S(Q,\omega) \cdot const. \end{aligned} \tag{33}$$

The final value theorem, stating that the signal at the origin in the frequency domain equals the signal area in the time domain , we have:

$$S_R(Q,\omega=0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} I(Q,t) \cdot R(Q,t) e^{-i\omega t} dt = \int_{-\infty}^{+\infty} I(Q,t) \cdot R(t) dt \tag{34}$$

and hence the measured scattering law $S_R(Q,\omega)$ reduces itself to a time average of $I(Q,t)R(t)$. A part from this ideal case, in the more general condition in which the resolution function in the ω-space has a nonegligible width, the experimentally measured elastic scattering law, due to the finite energy instrumental resolution $\Delta\omega$, $S_R^M(Q)$ is:

$$S_R^M(Q) = \int_{\frac{-\Delta\omega_{RES}}{2}}^{\frac{+\Delta\omega_{RES}}{2}} S_R(Q,\omega) d\omega \tag{35}$$

And hence,

$$
\begin{aligned}
S_R^M(Q) &= \int_{\frac{-\Delta\omega_{RES}}{2}}^{\frac{+\Delta\omega_{RES}}{2}} S(Q,\omega) \otimes_t R(Q,\omega) d\omega \\
&= \int_{\frac{-\Delta\omega_{RES}}{2}}^{\frac{+\Delta\omega_{RES}}{2}} \left[\frac{1}{\sqrt{2\pi}} I(Q,t) \cdot R(Q,t) e^{-i\omega t} dt \right] d\omega
\end{aligned}
\tag{36}
$$

For a given fixed instrumental energy resolution function $\Delta\omega_{RES}$one gets for the elastic contribution:

$$
\begin{aligned}
S_R^M(Q) &= \int_{\frac{-\Delta\omega_{RES}}{2}}^{\frac{+\Delta\omega_{RES}}{2}} \left[\frac{1}{2\pi} \int_{-\infty}^{+\infty} I(Q,t) \cdot R(Q,t)) cos(\omega t) dt \right] d\omega \\
&\approx S_R(Q,\omega = 0) \cdot \Delta\omega_{RES}
\end{aligned}
\tag{37}
$$

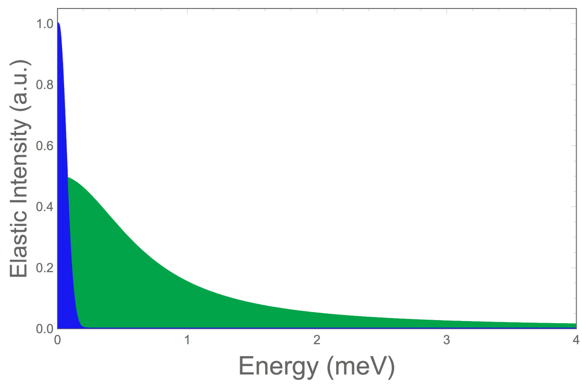

FIGURE 8. Elastic (blue) and quasi-elastic (green) contributions reflecting the long and short time system dynamics.

Figure 8 shows the elastic (blue) and quasi-elastic (green) contributions. The first one refers to the system dynamics that occurs on a time scale longer than the instrumental energy resolution whose contribution is entirely summed up in the elastic curve(Branca *et al.* 2004a,b; Maccarrone *et al.* 2004; Magazù *et al.* 2004a,d,e, 2006b). The second one refers to the system dynamics that occurs on a time scale shorter than the instrumental energy resolution whose contribution is weighted by the resolution function and gives rise to the quasi-elastic broader band (Branca *et al.* 2003a; Magazù *et al.* 2003, 2004c; Migliardo *et al.* 2004). In the following we will address our attention to an analysis of the time dependent pair correlation function in the long time regime, i.e. for times longer than the instrumental resolution time. Such a regime corresponds to the case of the elastic and quasi-elastic scattering, in this regime, introducing the instrumental resolution time τ' one has (Jannelli *et al.* 1996; Faraone *et al.* 1999; Magazù *et al.* 2001b; Branca *et al.* 2002a, 2005; Hennet *et al.* 2011):

$$\int_{\tau'}^{+\infty} G_R(r,t)dt = \int_{\tau'}^{+\infty} G(r,t) \cdot R(t)dt \tag{38}$$

From a general point of view, assuming that the pair correlation function $G(r,t)$ in the time domain is a Gaussian with a linewidth τ while the resolution function $R(r,t)$ in the time domain is a Gaussian with a linewidth of τ', then the $G_R(r,t)$matrix elements can be evaluated taking into account the $G(r,t)$ matrix elements with $\tau < \tau'$ Such elements are weighted by the resolution function $R(r,t)$. For longer times, i.e. for $\tau > \tau'$, all together the elements of $G(r,t)$ with $\tau > \tau'$ will contribute to the calculation furnishing a unique average value of $G_R(r,\tau > \tau')$ see Figure 9. This latter condition corresponds to the elastic scattering.

$G_R(1,1)$	$G_R(1,2)$	...	$G_R(i,j)$	...	$G_R(1,m;\tau < \tau')$	$G(1, \tau > \tau')$
$G_R(2,1)$						
...						
$G_R(i,1)$						
...						
$G_R(m-1,1)$						
$G_R(m,1)$						

τ'

FIGURE 9. $G_R(i,j)$ for $\tau > \tau'$.

Figure 10 reports the evaluation procedure of $G_R(r,t)$ for $\tau > \tau'$ by increasing τ'. Its value is furnished by the integrated area (in cyan) between the curve and the τ axis for $\tau > \tau'$.

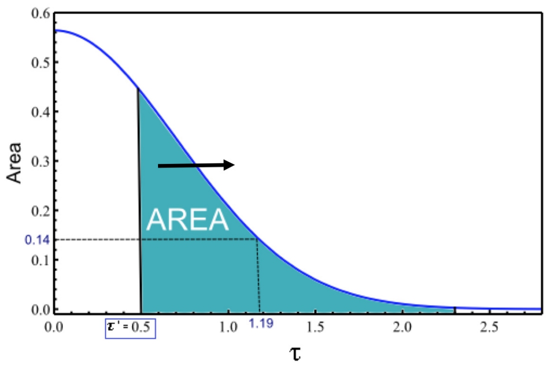

FIGURE 10. Evaluation procedure of for $\tau > \tau'$ by increasing τ'.

Finally, Figure 11 shows the evaluated integrated area of a Gaussian with a linewidth of $\tau = 1$ as a function of τ'.

To report a simple specific example, by applying the one point Gaussian quadrature rule, that is an approximation of the definite integral of a function, which allows to select both

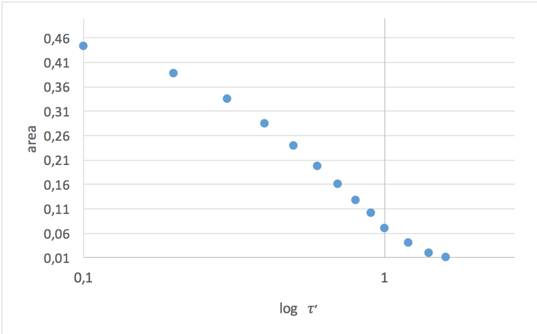

FIGURE 11. Evaluated integrated area of a Gaussian with a linewidth of $\tau = 1$ as a function of log τ'.

the weights and locations so that a higher order polynomial can be integrated (Schipke 1967; Gockenbach 2006), it is possible to extract a mean value for the integral function, i.e. $G_R(r, \tau > \tau')$for times longer in respect to τ' . In the specific case in which $a = \tau' = 0.5$ and $b = 2.3$:

$$\int_a^b f(x)dx \approx c_1 f(x_1) = (b-a)f\left(\frac{b+a}{2}\right) \tag{39}$$

it results that the average value of f$G_R(r,t)$ for $\tau > \tau'$corresponds to the value of $G(r,t)$ at $t \approx (1+0.19)\tau'$. We can conclude that the elements of the array associated to $G(r,t)$ with $\tau > \tau'$, which represents the linewidth of the time dependent resolution function, furnish an average value corresponding to $G(r, t \approx 1.19\tau')$. The present study puts into evidence that the component related to the instrumental window, i.e. for $\tau > \tau'$, can be expressed as a mean value of the PCF evaluated in proximity of the instrumental resolution time.

7. Conclusions

The present work reports an approach concerning the effects of a windowing of an energy zero centered signal within the formalism of the time dependent pair correlation functions. The system-probe interaction is dealt by taking into account the coupling between the system scattering law and the instrument energy resolution function in terms of convolution product. The introduced approach is developed also in terms of matrices. The case of separability of two dimensional functions is discussed. From the present analysis it emerges that the system dynamics that occurs on a time scale longer than the instrumental energy resolution, is entirely summed up in the elastic curve. On the other hand the system dynamics that occurs on a time scale shorter than the instrumental energy resolution is weighted by the resolution function and gives rise to the quasi-elastic broader band. One conclusion is that, as far as the measured scattering law is concerned, by changing the instrumental resolution one can register a crossover between a condition dominated by the elastic contribution to a condition dominated by the quasi-elastic contribution when the system relaxation time matches the instrumental resolution time. Furthermore, as far as the measured time dependent pair correlation function is concerned, the component related to the instrumental window can be connected with a mean value of the pair correlation function evaluated at a longer time in respect to the instrumental resolution time. The presented approach is applicable to the analysis of two dimensional zero-centered windowed signals where it is important to separate the time dependent contributions connected to the inside selected instrumental window from the unique value connected to the integral value of the time dependent contributions related to the outside selected instrumental window.

Appendix A. Fourier transforms and functions separability

It is well known that FT can be extended to n dimensions; in particular, a definition of FT for two dimensions is:

$$F(u,v) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y)e^{-2\pi i(ux+vy)dxdy} \tag{40}$$

and its inverse:

$$f(x,y) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} F(u,v)e^{2\pi i(ux+vy)dudv} \tag{41}$$

In general, FT is a complex function of the real frequency variables; as such the transform can be expressed in terms of its magnitude and phase. Some properties of FTs are summarized below:

- Linearity: The FT is a linear transform, taking into account two functions $f(x,y)$ and $g(x,y)$, with Fourier Transform given by $F(u,v)$ and $G(u,v)$, respectively, the FT of any linear combination of f and g can be found:

$$af(x,y)+bg(x,y) \Leftrightarrow aF(u,v)+bG(u,v) \tag{42}$$

- Shifting or Translation: A shift in position in one domain gives rise to a phase change in another domain. If the original function $f(x,y)$ is shifted in spatial coordinates, it should have the same magnitude and the same phase of the spectrum:

$$f(x-x_0,y-y_0)+bg(x,y) \Leftrightarrow e^{-2\pi i(ux_0+vy_0)}F(u,v) \tag{43}$$

- Modulation: Multiplication with a cosine has the effect of shifting the spectrum to center on the frequency of the cosine:

$$e^{2\pi i(ux_0+vy_0)}f(x,y) \Leftrightarrow F(u-u_0,v-v_0) \tag{44}$$

- Convolution: convolution in the spatial domain is equivalent to multiplication in the Fourier (frequency) domain and vice-versa:

$$f(x,y)\otimes g(x,y) \Leftrightarrow F(u,v)G(u,v) \tag{45}$$

- Multiplication

$$F(u,v)G(u,v) \Leftrightarrow f(x,y)\otimes g(x,y) \tag{46}$$

- Conjugation: If a 2D signal is real, then the Fourier transform has certain symmetries

$$f^*(x,y) = F(-u,-v) \tag{47}$$

- Separability:

$$f(x,y) = f(x)f(y) \Leftrightarrow F(u,v) = F(u)F(v) \tag{48}$$

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