New York University
Physics Department
Class GA.2061 "Non-Equilibrium Statistical Physics", Fall 2021

Home Work 05 *Solutions*

1. FDT (Fluctuation-Dissipation Theorem) relates generalized susceptibility (same as response function) $\chi(t)$, which describes the response of variable y to the force conjugate to variable x, and correlation function $\phi_{xy}(t)$:

$$\chi(t) = \begin{cases} -\frac{1}{T}\frac{d}{dt}\langle y(t)x(0)\rangle & \text{for} \;\; t > 0 \\ 0 & \text{for} \;\; t < 0 \end{cases} . \tag{1}$$

When both y and x are "coordinate-like" (i.e., do not change upon time reversal), then the equivalent formulation of FDT says

$$\chi''(\omega) = \frac{\omega}{2T}(yx)_\omega . \tag{2}$$

Derive similar result for the case when y is velocity-like (i.e., flips the sign upon time reversal).

Solution

The equation (1) remains unchanged. To switch to the frequency dependent quantities, we define, for both $t > 0$ and $t < 0$,

$$\beta(t) = -\frac{1}{T}\frac{d}{dt}\langle y(t)x(0)\rangle . \tag{3}$$

In case y is coordinate-like we have $\langle y(t)x(0)\rangle = \langle y(-t)x(0)\rangle$, which then means $\beta(t) = -\beta(-t)$ (because of time derivative). When y is velocity-like, we have the opposite: $\langle y(t)x(0)\rangle = -\langle y(-t)x(0)\rangle$, leading to $\beta(t) = \beta(-t)$. Moreover, $\beta(t)$ is obviously real.

Now as regards χ_ω, we have

$$\chi_\omega = \int_0^\infty \beta(t)e^{\imath\omega t}dt . \tag{4}$$

Therefore,

$$\chi_\omega^* = \underbrace{\int_0^\infty \beta(t)e^{-\imath\omega t}dt}_{\text{replace } t\to -t} = \int_{-\infty}^0 \beta(-t)e^{\imath\omega t}dt . \tag{5}$$

This leads to the conclusion that for coordinate-like y we have $\chi_\omega - \chi_\omega^* = \beta_\omega$, while for velocity like y the similar result reads $\chi_\omega + \chi_\omega^* = \beta_\omega$. In other words, $2\imath\chi_\omega'' = \beta_\omega$ for coordinate-like case and $2\chi_\omega' = \beta_\omega$ for velocity-like.

As regards β_ω, it is found from

$$\langle y(t)x(0)\rangle = \int_{-\infty}^\infty (yx)_\omega e^{-\imath\omega t}\frac{d\omega}{2\pi} \quad \Longrightarrow \quad \beta_\omega = \frac{\imath}{T}\omega(yx)_\omega . \tag{6}$$

Thus we arrive at the result

$$\begin{aligned} \chi_\omega'' &= \tfrac{\omega}{2T}(yx)_\omega \;\; \text{for coordinate} - \text{like } y \\ \chi_\omega' &= \tfrac{\imath\omega}{2T}(yx)_\omega \quad \text{for velocity} - \text{like } y \end{aligned} \tag{7}$$

while x is assumed coordinate-like in both cases. An important note: when y is velocity-like, we should realize that the presence of i does not mean that χ_ω' is imaginary, because in fact in this case $(yx)_\omega$ is imaginary.

Note that the usual statement relating χ'' to dissipation is only valid when y is coordinate-like.

2. Use FDT (Fluctuation-Dissipation Theorem) to derive

   (a) power spectrum of velocity fluctuations for a Brownian particle, taking into account inertia;

(b) power spectrum of velocity fluctuations for a slightly damped harmonic oscillator (i.e., for a Brownian particle with inertia, attached to an immobile point by a harmonic spring).

Show how weakly damped oscillator resonates to the part of thermal drive that is close to its own frequency.

Solution

Assuming $x(t)$ is particle coordinate, its motion under force $f(t)$ is described by $m\ddot{x} + \xi\dot{x} = f(t)$. In frequency representation, that means $(-m\omega^2 - \imath\xi\omega)x_\omega = f_\omega$, or $\chi_\omega = \frac{1}{-m\omega^2 - \imath\xi\omega}$. This can be re-written as $\chi_\omega = \frac{\imath\xi\omega - m\omega^2}{\xi^2\omega^2 + m^2\omega^4}$, from which the imaginary part is $\chi''_\omega = \frac{\xi\omega}{\xi^2\omega^2 + m^2\omega^4}$. Therefore, power spectrum of coordinate reads $\left(x^2\right)_\omega = \frac{2T}{\omega}\frac{\xi\omega}{\xi^2\omega^2 + m^2\omega^4}$. And since $v_\omega = -\imath\omega x_\omega$, we arrive at

$$(v^2)_\omega = 2T\frac{\xi}{\xi^2 + m^2\omega^2} \ . \tag{8}$$

Thus, this power spectrum is only quasi-flat at frequencies smaller than $\omega^\star = \xi/m$, but it is essentially truncated at larger frequencies. This exactly corresponds to the idea that the motion is ballistic at times shorter than $1/\omega^\star$ and diffusive at larger times.

Now the same story for a harmonic oscillator: $m\ddot{x} + \xi\dot{x} + kx = f(t)$. In frequency representation, that means $(-m\omega^2 - \imath\xi\omega + k)x_\omega = f_\omega$, or

$$\chi_\omega = \frac{1}{-m\omega^2 - \imath\xi\omega + k} = \frac{-m\omega^2 + \imath\xi\omega + k}{(-m\omega^2 - \imath\xi\omega + k)(-m\omega^2 + \imath\xi\omega + k)} \ . \tag{9}$$

Then $\chi''_\omega = \frac{\xi\omega}{\xi^2\omega^2 + (m\omega^2 - k)^2}$ and finally

$$(v^2)_\omega = 2T\frac{\xi\omega^2}{\left(m\omega^2 - k\right)^2 + \xi^2\omega^2} \ . \tag{10}$$

If damping ξ is small, this spectrum is sharply peaked at resonance frequency of the oscillator, $\omega = \sqrt{k/m}$: oscillator receives forcing on all frequencies but responds mostly on its own one.

The plot is in figure 1.

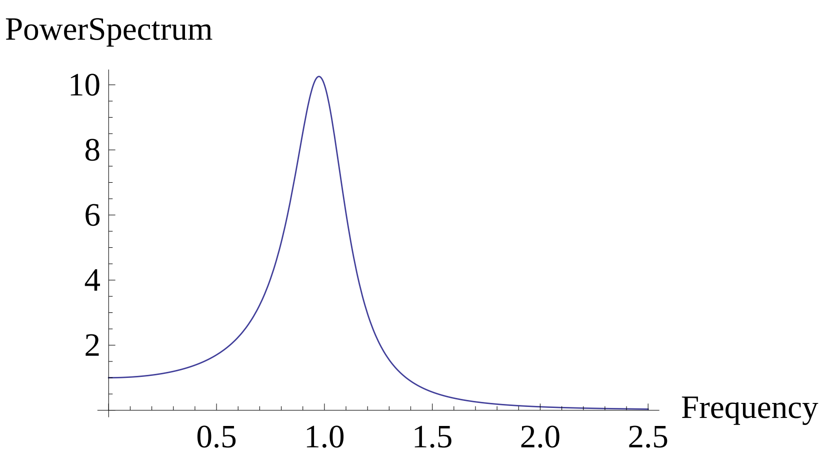

FIG. 1. The spectral density of fluctuations for a weakly damped harmonic oscillator. Horizontal axis is frequency in the units of resonant frequency, Frequency $= \frac{\omega}{\sqrt{k/m}}$, vertical axis is power spectrum in units such as $(x^2)_\omega \frac{k^2}{2T\xi}$, thus $(x^2)_\omega \frac{k^2}{2T\xi} = \frac{1}{(1-\varpi^2)^2 + (\xi^2/km)\varpi^2}$. The graph is plotted assuming $\xi^2/km = 0.1$. For problem 2.

Upon integration over all frequencies power spectrum $(x^2)_\omega$ has to give the equilibrium fluctuation of x:

$$\int_{-\infty}^{\infty} \left(x^2\right)_\omega \frac{d\omega}{2\pi} = \left\langle x^2 \right\rangle \ , \tag{11}$$

and the latter quantity is known to us from the equipartition theorem of classical statistics, $(k/2)\left\langle x^2\right\rangle = T/2$. Thus, we have to show that

$$\int_{-\infty}^{\infty} \frac{2T\xi}{(k-m\omega^2)^2+\xi^2\omega^2}\frac{d\omega}{2\pi} = \frac{T}{k} \quad \Longrightarrow \quad \int_{-\infty}^{\infty} \frac{1}{(k-m\omega^2)^2+\xi^2\omega^2} d\omega = \frac{\pi}{k\xi} \ . \tag{12}$$

The rest is pure mathematics, although relatively cumbersome. For reasons which I do not understand, *Mathematica* refuses to evaluate this integral – but it can be done by hand.

Integration, method 1:

The idea is to consider ω as a complex variable. To begin with, $(x^2)_\omega$ has four poles, as is seen from formula (9): two of them arise from the poles of α_ω, and two others are poles of α_ω^*. Looking at the quadratic equation $1/\alpha_\omega = 0$, we find the two poles of α_ω at complex frequencies

$$\omega_1 = \frac{\sqrt{4km-\xi^2}}{2m} - \imath\frac{\xi}{2m} \quad \text{and} \quad \omega_2 = -\frac{\sqrt{4km-\xi^2}}{2m} - \imath\frac{\xi}{2m} \ , \tag{13}$$

both having negative imaginary parts, i.e., both poles are located in the lower half-plane, as it must be to obey causality. I assumed here that $\xi < 2\sqrt{km}$, which is definitely true for sharply resonant system. Overall, our integrand in formula (12) has four poles, two pairs of complex conjugated ones; therefore, the integral can be written as

$$\int_{-\infty}^{\infty} \frac{1}{(k-m\omega^2)^2+\xi^2\omega^2} d\omega = \frac{1}{m^2}\int_{-\infty}^{\infty} \frac{1}{(\omega-\omega_1)(\omega-\omega_2)(\omega-\omega_1^*)(\omega-\omega_2^*)} d\omega \ . \tag{14}$$

It is now evident how to address this integral: integration contour can be completed through either upper or lower arch, yielding in either case just two residues:

$$\int_{-\infty}^{\infty} \frac{1}{(k-m\omega^2)^2+\xi^2\omega^2} d\omega = \frac{2\pi\imath}{m^2}\left[\frac{1}{(\omega_1-\omega_2)(\omega_1-\omega_1^*)(\omega_1-\omega_2^*)} + \frac{1}{(\omega_2-\omega_1)(\omega_2-\omega_1^*)(\omega_2-\omega_2^*)}\right] \ . \tag{15}$$

The rest is just the routine algebra, which yields the expected result (12).

Integration, method 2: Since the oscillator is sharply resonant, we can address the integral approximately, using the fact that ξ is in proper sense small, namely, $\xi \ll \sqrt{km}$. In this case the integrand has two very sharp peaks, at $\omega = \pm\sqrt{k/m}$, and the vicinities of those peaks dominate the integral. For instance, in the vicinity of the positive $\sqrt{k/m}$ we can write $\omega = \sqrt{k/m} + \delta$ and then

$$|\alpha_\omega|^2 = \frac{1}{\left(-2\delta\sqrt{km} - \underbrace{m\delta^2}\right)^2 + \left(\xi\left(\sqrt{k/m} + \underbrace{\delta}\right)\right)^2} \ . \tag{16}$$

The integral will be dominated by the region of such δ which is up to $\left(\delta\sqrt{km}\right)^2 \sim \xi^2$. In this region, since $\xi \ll \sqrt{km}$, the underbraced terms can be neglected compared at the terms next to them:

$$|\alpha_\omega|^2 \simeq \frac{1}{\left(-2\delta\sqrt{km}\right)^2 + \left(\xi\left(\sqrt{k/m}\right)\right)^2} \ . \tag{17}$$

This yields elementary integral, and since there are two peaks we get the same answer as before

$$\int_{-\infty}^{\infty} |\alpha_\omega|^2 d\omega \simeq 2\int_{-\infty}^{\infty} \frac{1}{\left(-2\delta\sqrt{km}\right)^2 + \left(\xi\left(\sqrt{k/m}\right)\right)^2} d\delta = \frac{2}{k\xi}\int_{\infty}^{\infty} \frac{dx}{1+x^2} = \frac{\pi}{k\xi} \ . \tag{18}$$

3. One important realization of the "response function" has to do with rheology – the study of mechanical properties of materials. Consider a planar slab of material and suppose that we subject it to a constant shear stress $\sigma = f/A$, where f is shearing force and A is surface area. If the sample is solid, then shear strain $\gamma = \Delta x/h$ is linear in the applied stress: $\sigma = G\gamma$, where δx is how far the upper surface moved compared to the lower one, h is the thickness of the slab, and G is the shear modulus. On the other hand, if the sample is liquid, then shear *rate* $\dot\gamma$ is linear in the applied stress: $\dot\gamma = \sigma/\eta$, where η is viscosity. Many real materials exhibit elastic response at

large frequencies and viscous response at small frequencies. Maxwell suggested a simple model which has this property: imagine a sandwich with a layer of liquid (e.g., mayonnaise) of thickness h_1 sitting on top of a layer of solid (e.g., bread) of thickness h_2, with $h_1 + h_2 = h$. Work out the relaxation of stress in Maxwell model after a step strain ("switch on" experiment). Along with relaxation modulus $G(t)$, find also its Fourier transform $\tilde{G}_\omega$ as well as complex modulus G_ω; how are these two quantities related to one another [1]?

Solution

The physical idea is that when strain is imposed very rapidly, the elastic part gets stressed, while the viscous part does not have time to react and remains at (almost) zero strain. Then, the viscous part slowly moves to allow the elastic part to relieve its stress which eventually goes to zero and disappears. In the end I will discuss how rapidly should we impose the strain.

For the sandwich-like structure, the displacements add together at every moment

$$h_v \gamma_v(t) + h_e \gamma_e(t) = h\gamma(t) \ , \tag{19}$$

where h_v and h_e are the thicknesses of viscous and elastic parts, respectively; $h_v + h_e = h$. This relation must hold at all times. And the stress must be the same everywhere, which means

$$\sigma(t) = G\gamma_e = \eta\dot{\gamma}_v \ . \tag{20}$$

This combines into a differential equation

$$\dot{\sigma} = -\frac{G}{\eta}\frac{h_e}{h_v}\sigma(t) \ . \tag{21}$$

The initial condition for this is that the initial strain in viscous part is zero, or

$$\gamma_v\big|_{t=0} = 0 \quad \Longrightarrow \quad \gamma_e\big|_{t=0} = \frac{h}{h_e}\gamma \quad \Longrightarrow \quad \sigma\big|_{t=0} = G\frac{h}{h_e}\gamma \ . \tag{22}$$

With this we obtain

$$\sigma(t) = G\frac{h}{h_e}\gamma e^{-t/\tau} \ , \quad \text{where} \quad \tau = \frac{\eta}{G}\frac{h_v}{h_e} \ . \tag{23}$$

Importantly, as soon as there is both elastic (G) and viscous (η) response in the system - there is also a new time scale, which is τ. Over this time, the viscous part allows the relaxation of stress in the elastic part.

This sheds light also on the "instant" application of the initial strain. The stress in the solid equilibrates with the speed of sound, let us call it s, which means its characteristic time scale is h_e/s. The consideration above makes sense as long as $h_e/s \ll \tau$ – which of course is the case for most real materials.

Assuming $G(t) = G_0 e^{-t/\tau}$ at $t > 0$ and 0 at $t < 0$, Fourier transform reads $\tilde{G}_\omega = \frac{G_0\tau}{1-i\omega\tau}$ (pole is in the lower half plane, as it should be).

In general the relation between $\tilde{G}_\omega$ and G_ω is this:

$$\tilde{G}_\omega = \frac{i}{\omega}G_{-\omega} \quad \text{equivalently} \quad \begin{array}{l} \tilde{G}'_\omega = \frac{1}{\omega}G''_\omega \\ \tilde{G}''_\omega = \frac{1}{\omega}G'_\omega \end{array} \ . \tag{24}$$

Indeed, if we have oscillatory strain $\gamma(t) = \gamma_0 e^{i\omega t}$, then our stress will be $G_\omega \gamma_0 e^{i\omega t}$ (this is the definition of complex modulus). On the other hand, strain rate will be $\dot{\gamma}(t) = \gamma_0 i\omega e^{i\omega t}$ and then stress is $\int G(t-t')\dot{\gamma}(t')dt' = \int G(t-t')\gamma_0 i\omega e^{i\omega t'}dt' = \gamma_0 i\omega e^{i\omega t}\tilde{G}_{-\omega}$.

Therefore, complex modulus for the Maxwell model reads

$$G_\omega = G_0\frac{i\omega\tau}{1+i\omega\tau} \quad \Longrightarrow \quad \begin{array}{l} G'_\omega = G_0\frac{(\omega\tau)^2}{1+(\omega\tau)^2} \\ G''_\omega = G_0\frac{\omega\tau}{1+(\omega\tau)^2} \end{array} \tag{25}$$

where storage G'_ω and loss G''_ω moduli are the real and imaginary parts of the complex modulus. The corresponding plots are in Figure 2.

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[1] The relation between these two quantities is quite general, valid not only for Maxwell model.

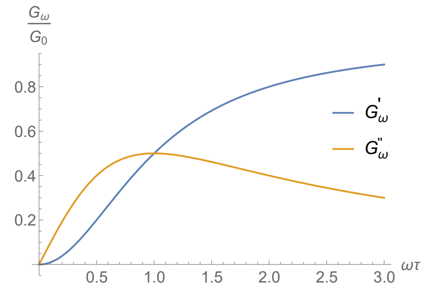

FIG. 2. Storage G'_ω and loss G''_ω moduli as functions of frequency for the Maxwell model. At low frequency, $G''_\omega > G'_\omega$, which means the response is predominantly viscous, while at large frequency the opposite inequality holds, $G''_\omega < G'_\omega$, which means the response is predominantly elastic.

4. Consider paper [1] (see also their earlier work [2]) and answer, one by one, the following questions. Authors used FDT; what did they use it for, what did they find out? FDT is a statement of equality of two quantities, which of them did they measure? Did authors check that the observed fluctuations are within linear response regime? Did they have to check it? What did they check about linear response and how? What is the characteristic frequency below which non-thermal drive is observed? In figure 2, a and b, the plot (by empty symbols) the quantity $C(f)\pi f/k_BT$; what is it? Does the coefficient agree with FDT formulation obtained in class?

Solution

Authors performed two different experiments, in one they passively measured fluctuations, in the other they actively exerted force and measured response; thus, they measured *both* sides of the FDT relation. FDT is valid for equilibrium systems, it describes thermally driven fluctuations around equilibrium state. By observing deviations from FDT, authors have proven that red blood cell is not an equilibrium system, and that part if its fluctuations is not thermally driven. Deviations are seen below roughly 10 Hz. They did not have to check the smallness of fluctuations, but they did check that the response was linear in the driven experiment. FDT does not involve the assumption that fluctuations are small; it says that correlation functions of fluctuations, whatever they are, is related to the linear response function.

The coefficient $\pi f/k_BT$ is exactly the same as what we had $\omega/2T$, because $\omega = 2\pi f$ and we used different units for temperature.

5. Find power spectrum of transverse velocity fluctuations in an infinite volume of an incompressible fluid.

Hint 1: Equation of motion for a fluid is quite complex, it is called Navier-Stokes equation. For an incompressible fluid, it is significantly simplified. And if we are only interested in transverse velocity, then the equation is simplified even further[2]:

$$\frac{\partial \mathbf{v}^\perp}{\partial t} = \frac{\eta}{\rho}\nabla^2 \mathbf{v}^\perp \ . \tag{26}$$

Here ρ is the liquid density, and η viscosity; the ratio η/ρ is sometimes called kinematic viscosity.

Hint 2: Correlation function $\left\langle v^\perp_\alpha(t,\mathbf{r}) v^\perp_\beta(t',\mathbf{r}')\right\rangle$ depends only on the differences $t-t'$ and $\mathbf{r}-\mathbf{r}'$. That means, in terms of Fourier transforms, defined here as $v^\perp_{\alpha\mathbf{k}\omega} = \int dt d^3\mathbf{r} e^{\imath\omega t - \imath\mathbf{k}\mathbf{r}} v^\perp_\alpha(t,\mathbf{r})$, correlation function must read

$$\left\langle v^\perp_{\alpha\mathbf{k}\omega} v^\perp_{\beta\mathbf{k}'\omega'}\right\rangle = (2\pi)^4\delta(\omega+\omega')\delta(\mathbf{k}+\mathbf{k}')\left(v^\perp_\alpha v^\perp_\beta\right)_{\mathbf{k}\omega} \ , \tag{27}$$

where $\left(v^\perp_\alpha v^\perp_\beta\right)_{\mathbf{k}\omega}$ is a new function of one frequency ω and one wave vector $\mathbf{k}$; this is exactly the power spectrum you have to find. According to Wiener-Khinchin theorem, power spectrum in question is nothing else but Fourier transform of the correlation function.

[2] For your information, here is the Navier-Stokes equation for an incompressible fluid:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathrm{v}\cdot\nabla)\,\mathrm{v} = -\frac{1}{\rho}\nabla p + \frac{\eta}{\rho}\nabla^2\mathbf{v} \ ,$$

where p is hydrostatic pressure. You may want to exercise separating here the transverse component. If you want to do it, you should present velocity as a sum of transverse and longitudinal components, $\mathbf{v} = \mathbf{v}^\perp + \mathbf{v}^\parallel$, such that div $\mathbf{v}^\perp = 0$ and curl $\mathbf{v}^\parallel = 0$

Hint 3: Correlation function $\left\langle v_\alpha^\perp(t,\mathbf{r}) v_\beta^\perp(0,\mathbf{0})\right\rangle$ is defined in the usual way for $t > 0$ and is continued based on symmetry properties to $t < 0$.

Hint 4: There is a useful mathematical trick, described for you below in the Appendix A.

Solution

According to Wiener-Khinchin theorem, power spectrum in question is nothing else but Fourier transform of the correlation function. This is what we need to find.

Equation of motion – Navier-Stokes equation – for the transverse velocity in an incompressible fluid is reduced to

$$\frac{\partial \mathbf{v}^\perp}{\partial t} = \frac{\eta}{\rho}\nabla^2 \mathbf{v}^\perp \ . \tag{28}$$

Note that the dynamics equation above has the form of a diffusion equation, and kinematic viscosity η/ρ has dimension of a diffusion coefficient; this equation describes diffusion of momentum. Correlation function of transverse velocities, as usual, must satisfy the same equation at $t > 0$:

$$\frac{\partial \left\langle v_\alpha^\perp(t,\mathbf{r}) v_\beta^\perp(0,0)\right\rangle}{\partial t} = \frac{\eta}{\rho}\nabla^2 \left\langle v_\alpha^\perp(t,\mathbf{r}) v_\beta^\perp(0,0)\right\rangle \ . \tag{29}$$

To solve it, we first can perform Fourier transform with respect to coordinates $\mathbf{r}$, this replaces Laplacian in the right hand side with $-\mathbf{k}^2$ and thus our equation becomes exactly of the form described in the Appendix A, with $\lambda \to \eta k^2/\rho$. Although velocity has time reversal signature of -1, the correlation function in question is between two velocities, which is why correlation function of velocities must be an even function of time. Therefore,

$$\left(v_\alpha^\perp v_\beta^\perp\right)_{\mathbf{k}\omega} = \frac{2\eta k^2/\rho}{(\eta k^2/\rho)^2 + \omega^2}\left(v_\alpha^\perp v_\beta^\perp\right)_{\vec{k}} \ . \tag{30}$$

The last factor $\left(v_\alpha^\perp v_\beta^\perp\right)_{\vec{k}}$ plays the role of $\phi(0)$, this is an equilibrium (simultaneous) average, we have found it before. Plugging here the simultaneous correlation which we found before, we get

$$\left(v_\alpha^\perp v_\beta^\perp\right)_{\omega\mathbf{k}} = \frac{T}{\rho}\left(\delta_{\alpha\beta} - \frac{k_\alpha k_\beta}{k^2}\right)\frac{\frac{\eta}{\rho}k^2}{\left(\frac{\eta}{\rho}\right)^2 k^4 + \omega^2} \tag{31}$$

The problems below are not required and will not be graded, but recommended to those students who want to improve their knowledge and performance.

6. Addressing spectral decomposition of fluctuations, we defined Fourier transforms as follows:

$$f_\omega = \int_{-\infty}^{+\infty} f(t)e^{\imath\omega t}dt \ , \quad f(t) = \int_{-\infty}^{\infty} f_\omega e^{-\imath\omega t}\frac{d\omega}{2\pi} \ . \tag{32}$$

In reality, we never have access to any quantity $f(t)$ over an infinite interval of time, nor do we measure spectrum f_ω over an infinite bandwidth of frequencies. Similar constraint also exists when we are talking about spatial dependencies, $f(x)$, and corresponding Fourier transforms, f_k. Imagine, therefore, that you have some $2N$ data points spread over finite period of time T or finite length L, each point sitting in the middle of the interval Δt or Δx; $T = 2N\Delta t$ or $L = 2N\Delta x$ (it is unimportant, but convenient to consider an even number of points, hence $2N$). How would you define corresponding discrete Fourier transform? How many frequencies will be presented? What will be the bandwidth? How would you define the continuous limit of Fourier transforms? How would you formulate Wiener-Khinchin theorem in discrete case?

Solution

Suppose our function is known (measured) in points $x_n = \left(n + \frac{1}{2}\right)\Delta x$, for $-N \le n \le N-1$; it is convenient to choose them symmetrically positioned around zero, at $\pm\frac{\Delta x}{2}$, $\pm\frac{3\Delta x}{2}$, $\pm\frac{5\Delta x}{2}$, etc. Each point is positioned in the middle of the interval Δx, and so the total length is $L = 2N\Delta x$; see Fig. 3. The smallest wave number we can possibly detect is $2\pi/L$, while the largest is $2\pi/\Delta x$. We therefore have $2N$ values of k, it is convenient to place them symmetrically between $-\pi/\Delta x$ and $\pi/\Delta x$. Those who know solid state physics will recognize this as Brillouin zone. There are $2N$ uniformly spaced values of k in this Brillouin zone, with interval $\Delta k = \frac{2\pi}{L}$, so that $k_p = \left(p + \frac{1}{2}\right)\Delta k$, with p integer, $-N \leq p \leq N-1$. The number of representative frequencies, k_p, is $2N$, exactly the same as the number of points x_n; it is very important, because Fourier transform does not add or loose any information encoded in the measured values $f(x_n)$.

In what follows, instead of writing sums over n (in real space) or over p (in reciprocal k space):

$$\sum_{n=-N}^{N-1} \ldots = \sum_{x=-L/2}^{L/2} \ldots \qquad \sum_{p=-N}^{N-1} \ldots = \sum_{k=-\pi/\Delta x}^{\pi/\Delta x} \ldots . \tag{33}$$

Then we can take our function $f(x)$, which we know in $2N$ points x_n, and consider the following sum:

$$\tilde{f}_{k_p} = \sum_{n=-N}^{N-1} e^{\imath k_p x_n} f(x_n) \equiv \sum_x e^{\imath k_p x} f(x) . \tag{34}$$

So far it is only a notation, but we need to establish that we can reconstruct $f(x)$ if we know $\tilde{f}_{k_p}$. To see this, multiply both sides of Eq. (34) by $e^{-\imath k_p x_m}$ and perform the sum over all possible wave numbers, i.e., over all p:

$$\begin{aligned} \sum_{p=-N}^{N-1} e^{-\imath k_p x_m} \tilde{f}_{k_p} &= \sum_{p=-N}^{N-1} \sum_{n=-N}^{N-1} e^{\imath k_p (x_n - x_m)} f(x_n) = \\ &= \sum_{n=-N}^{N-1} f(x_n) \left[\underbrace{\sum_{p=-N}^{N-1} e^{\imath k_p (x_n - x_m)}}_{2N\delta_{n,m}} \right] = 2N f(x_m) \end{aligned} . \tag{35}$$

The key here is the expression in square brackets, which turns out to be the Kronecker δ: it is a wonderful fact that plain waves $e^{\imath kx}$ are orthogonal not only over an infinite continuous interval, but also over the discrete set of points [3]. Thus, instead of the continuous Fourier transform (34), we have now the discrete version:

$$\tilde{f}_k = \sum_x e^{\imath kx} f(x) , \qquad f(x) = \frac{1}{2N} \sum_k e^{-\imath kx} \tilde{f}_k , \tag{36}$$

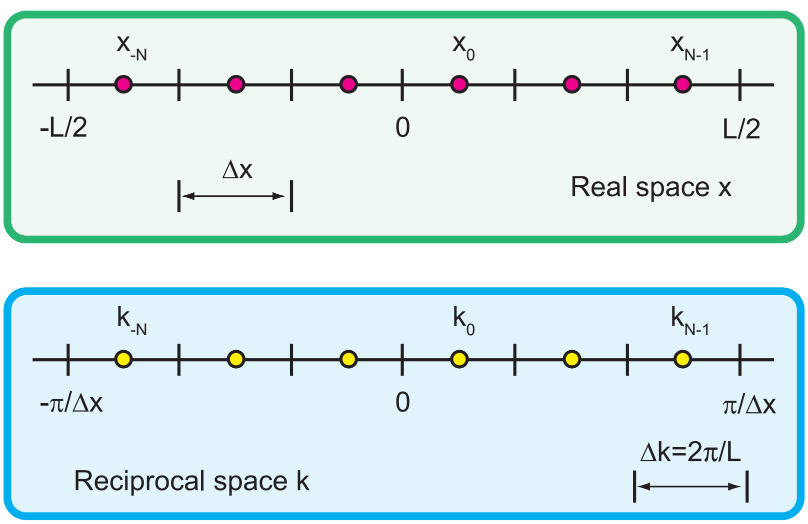

FIG. 3. Positioning of points x_n in real space, symmetrically around 0, and also of points k_p in the reciprocal space in Brillouin zone, also symmetrically around 0.

[3] It is useful to see that this is indeed the Kronecker δ. For this purpose, first of all, note that at $x_n = x_m$ the sum trivially reduced to $2N$. Further, if $x_n \neq x_m$, plug in the above expressions for k_p and x_n and see that the expression in square brackets gets reduced to the sum of a geometric series: $r^{1/2} \sum_{p=-N}^{N-1} r^p = \frac{r^N - r^{-N}}{r^{1/2} - r^{-1/2}}$, where $r = e^{\imath \frac{\pi}{2} \frac{n-m}{N}}$, which reduces to $1 - e^{2\pi\imath(n-m)} = 0$, as long as $n - m$ is an integer.

where x runs over discrete set of points $x_n = \left(n+\frac{1}{2}\right)\Delta x$, and k runs over discrete set of the same number of points $k_p = \left(p+\frac{1}{2}\right)\Delta k$, and $\Delta k = 2\pi/L$, as stated before; see again Fig. 3. Very importantly, while the interval along x depends on how many points you sample, N, the interval along k depends on the size of your system, L. Accordingly, if you take $N \to \infty$ and $L \to \infty$, you can replace summation by integrals

$$\sum_{n=-N}^{N-1} \ldots \simeq \int_{-L/2}^{L/2} \ldots \frac{dx}{\Delta x} \quad \text{and} \quad \sum_{k=-\pi/\Delta x}^{\pi/\Delta x} \ldots = \int_{-\pi/\Delta x}^{\pi/\Delta x} \ldots \frac{dk}{\Delta k} \ , \tag{37}$$

which means

$$\tilde{f}_k = \frac{2N}{L}\int_{-L/2}^{L/2} e^{\imath kx} f(x) \ , \qquad f(x) = \int_{-2\pi N/L}^{2\pi N/L} e^{-\imath kx} \frac{L}{2N} \tilde{f}_k \frac{dk}{2\pi} \ , \tag{38}$$

which comes back to our standard case (34) upon renaming $\frac{L}{2N}\tilde{f}_k \to f_k$, provided that N goes to infinity faster than L, which means sampling becomes better, not worse. Note that by the same token also

$$\sum_{k=-\pi/\Delta x}^{\pi/\Delta x} e^{\imath k(x_n - x_m)} = 2N\delta_{x_n,x_m} \quad \longrightarrow \quad \int_{\pi/\Delta x}^{\pi/\Delta x} e^{\imath k(x_n-x_m)} \frac{dk}{2\pi} = \frac{1}{\Delta x}\delta_{x_n,x_m} \to \delta(x_n - x_m) \ . \tag{39}$$

Returning now to Wiener-Khinchin theorem, we want correlation function $\langle f(x)f(y)\rangle$ to depend only on $x-y$. We plug in $f(x)$ and $f(y)$ in terms of the discrete Fourier transform, and get

$$\langle f(x)f(y)\rangle = \frac{1}{(2N)^2}\sum_{k,k'} e^{-\imath kx - \imath k' y}\left\langle \tilde{f}_k \tilde{f}_{k'}\right\rangle \ . \tag{40}$$

For this to depend only on $x-y$, the quantity $\left\langle \tilde{f}_k \tilde{f}_{k'}\right\rangle$ must be zero unless $k = -k^{-\prime}$, which means $\left\langle \tilde{f}_k \tilde{f}_{k'}\right\rangle = \left\langle \tilde{f}_k \tilde{f}_{-k}\right\rangle \delta_{k,-k'}$. Since $f(x)$ is real, it follows that $\tilde{f}_{-k} = \tilde{f}_k^{\star}$. Therefore,

$$\left\langle \tilde{f}_k \tilde{f}_{k'}\right\rangle = \left\langle \left|\tilde{f}_k\right|^2\right\rangle \delta_{k,-k'} \ . \tag{41}$$

Plug this into Eq. (40):

$$\langle f(x')f(x'+x)\rangle = \frac{1}{(2N)^2}\sum_{k} e^{-\imath kx}\left\langle \left|\tilde{f}_k\right|^2\right\rangle \ . \tag{42}$$

Compare this with the definition of discrete Fourier transform (36), we see that $\left\langle \left|\tilde{f}_k\right|^2\right\rangle/2N$ is actually the discrete Fourier transform of correlation function:

$$\frac{1}{2N}\left\langle \left|\tilde{f}_k\right|^2\right\rangle = \sum_{x}\langle f(0)f(x)\rangle\, e^{\imath kx} \ . \tag{43}$$

This is the discrete analog of Wiener-Khinchin theorem. To make it even more transparent, remember that $\tilde{f}_k = (2N/L)f_k$, while summation over x can be replaced by the integral $\sum_x \ldots = \int \ldots \frac{dx}{\Delta x}$ ($\Delta x = L/2N$), which leads to

$$\frac{1}{L}\left\langle |f_k|^2\right\rangle \simeq \int_{-L/2}^{L/2}\langle f(0)f(x)\rangle\, e^{\imath kx} dx \ , \tag{44}$$

and the right hand side, according to the regular Wiener-Khinchin theorem, is nothing else but the power spectrum $\left(f^2\right)_k$. Thus, finally

$$\boxed{\frac{1}{L}\left\langle |f_k|^2\right\rangle = \left(f^2\right)_k} \ . \tag{45}$$

This explains several important points: In practice, dealing with a finite system, you should consider "power spectrum" as simply $\langle f_k f_{-k}\rangle$, but you should expect it to grow linearly with the system size, and you may want to take it per unit length (or per unit time).

Appendix A: A useful mathematical trick

Suppose you want to find a correlation function $\phi(t)$. You define it at $t > 0$, where it satisfies some differential equation, for instance

$$\dot{\phi} = -\lambda\phi(t) \quad \text{at} \quad t > 0 \ . \tag{A1}$$

We usually solved it, and then continued solution for $t < 0$ based on the symmetry properties. And then, once the continuation is done, and once we knew $\phi(t)$ for all t, positive and negative, we could find its Fourier transform ϕ_ω, power spectrum, etc.

But in some of the more complex cases, it might be advantageous to solve this using the following method (which is sometimes called one-sided, or uni-lateral, Fourier transform, and is also closely related to the Laplace transform). Let us multiply both sides of equation (A1) by $e^{\imath\omega t}$ and integrate over *positive* t from 0 to infinity (i.e., only over those t where we know $\phi(t)$ and do not need symmetry continuation). In the left hand side, perform integration by parts:

$$\begin{aligned} \int_0^\infty e^{\imath\omega t}\dot{\phi}dt &= e^{\imath\omega t}\phi(t)\Big|_0^\infty - \imath\omega\int_0^\infty e^{\imath\omega t}\phi(t)dt \\ &= -\phi(0) - \imath\omega\int_0^\infty e^{\imath\omega t}\phi(t)dt \ . \end{aligned} \tag{A2}$$

In the right hand side, similar looking integral appears also. Let us denote it, say, as

$$\phi_\omega^+ = \int_0^\infty e^{\imath\omega t}\phi(t)dt \ , \tag{A3}$$

where superscript "+" serves as a reminder that integration runs over positive t only. In terms of this notation, we get

$$-\phi(0) - \imath\omega\phi_\omega^+ = -\lambda\phi_\omega^+ \quad \Longrightarrow \quad \phi_\omega^+ = \frac{\phi(0)}{\lambda - \imath\omega} \ . \tag{A4}$$

Can we use this result to find the Fourier transform, ϕ_ω? Yes, we can:

$$\begin{aligned} \phi_\omega = \int_{-\infty}^\infty e^{\imath\omega t}\phi(t)dt = \int_{-\infty}^0 e^{\imath\omega t}\phi(t)dt + \int_0^\infty e^{\imath\omega t}\phi(t)dt &= \int_0^\infty e^{-\imath\omega t}\phi(-t)dt + \int_0^\infty e^{\imath\omega t}\phi(t)dt \\ &= \pm\int_0^\infty e^{-\imath\omega t}\phi(t)dt + \int_0^\infty e^{\imath\omega t}\phi(t)dt \\ &= \pm\phi_{-\omega}^+ + \phi_\omega^+ \ , \end{aligned} \tag{A5}$$

where in the $\pm$ upper sign $+$ is for $\phi(t)$ even while lower sign $-$ for odd.

Combining, we find

$$\phi_\omega = \begin{cases} \frac{\phi(0)}{\lambda - \imath\omega} + \frac{\phi(0)}{\lambda + \imath\omega} = \frac{2\lambda\phi(0)}{\lambda^2+\omega^2} \text{ for } \phi(t) \text{ even} \\ \\ \frac{\phi(0)}{\lambda - \imath\omega} - \frac{\phi(0)}{\lambda + \imath\omega} = \frac{2\imath\omega\phi(0)}{\lambda^2+\omega^2} \text{ for } \phi(t) \text{ odd} \end{cases} \tag{A6}$$

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