Time-Dependent Statistical Mechanics
A1. The Fourier transform

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1 Definition of the Fourier transform and its inverse.

Suppose $F(t)$ is some function of time. Then its Fourier tranform with respect to time is defined as[1]

$$\hat{F}(\omega) \equiv \int_{-\infty}^{\infty} dt\, e^{i\omega t} F(t) \tag{1}$$

There are various definitions of the Fourier transform that differ in trivial ways. This is the one that is used most often in theoretical physics and chemistry. Note:

- there are no factors of 2π or $(2\pi)^{1/2}$ in front of the integral or in the exponent;
- we are using a complex exponential rather than a real sine or cosine;
- the sign in the exponent is positive.

A remarkable feature of the Fourier transform, which is a function of frequency ω, is that the function $F(t)$ can be reconstructed from the Fourier transform $\hat{F}(\omega)$ by an integration similar to that in the definition of the

[1]In these notes we shall be concerned only with the case that t and ω are real times and frequencies, respectively. In other contexts, the extensions of these results to the case of complex t and complex ω is very important.

Fourier transform.

$$F(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega t} \hat{F}(\omega) \tag{2}$$

This is an inverse Fourier transform, and the theorem that proves this result is called the Fourier integral theorem. Note the similarities and differences as compared with the Fourier transform.

- there is an additional factor of $1/2\pi$;
- the sign of the exponent is different.

Many of the functions that we deal with are finite and continuous functions of time, and they approach zero rapidly enough for large positive and negative times that the integral in Eq. (1) converges absolutely for all real ω. In such cases, the Fourier integral theorem holds as written. It is also correct, with some modification, under much less stringent conditions.[2] Here we note only two generalizations of the statement.

- If the integrals in (1) and (2) do not converge separately at the upper and lower limits, they are to be interpreted as

  $$\lim_{T \to \infty} \int_{-T}^{T} dt \, e^{i\omega t} F(t)$$

  and

  $$\lim_{\Omega \to \infty} \int_{-\Omega}^{\Omega} d\omega \, e^{-i\omega t} \hat{F}(\omega)$$

  respectively.
- If the function $F(t)$ is piecewise continuous, then Eq. (2) should be

  $$\lim_{\epsilon \to 0} \frac{1}{2} \left(F(t+\epsilon) + F(t-\epsilon) \right) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \, e^{-i\omega t} \hat{F}(\omega)$$

Exercise 1. Suppose

$$F_1(t) = A e^{-b|t|}$$

Calculate $\hat{F}_1(\omega)$.

[2] For a more detailed discussion and precise statements of the theorem, see Apostol or Titschmarch.

Exercise 2. Suppose

$$F_2(t) = Ae^{-b|t|} \cos \omega_0 t$$

Calculate $\hat{F}_2(\omega)$.

2 Elementary properties of the Fourier transform

1. The Fourier transform of a linear combination of functions is the linear combination of Fourier transforms; i.e. the Fourier tranform of $aF(t) + bG(t)$ is $a\hat{F}(\omega) + b\hat{G}(\omega)$.

2. If $F(t)$ is a real symmetric function of time (i.e. if $F(t) = F(-t)$ and F is real, for all real t) then $\hat{F}(\omega)$ is real for all real ω.

3. Consider a function, $F(t)$, and another function of time $G(t)$, which is defined as the function F shifted by an amount a along the time axis; i.e.
$$G(t) \equiv F(t - a)$$
Then
$$\hat{G}(\omega) = e^{i\omega a} \hat{F}(\omega)$$

4. Consider a function $F(t)$ and another function of time $G(t)$ that is defined as
$$G(t) \equiv e^{-i\omega_0 t} F(t)$$
Then
$$\hat{G}(\omega) = \hat{F}(\omega - \omega_0)$$

There is an interesting reciprocity between the last two of these statements. The third property states that shifting a function of time by an amount a along the time axis is equivalent to multiplying its Fourier transform by $\exp(i\omega a)$. The fourth property states that shifting the Fourier transform by an amount ω_0 on the frequency axis is equivalent to multiplying the inverse Fourier transform by $\exp(-i\omega_0 t)$.

Exercise 3. Prove these four statements from the definitions of the Fourier transform and the inverse Fourier transform.

Exercise 4. Get the answer to Exercise 2 using one or more of these principles.

3 Location and width of maxima in a Fourier transform.

As we shall discuss later in the course, an absorption spectrum is closely related to the Fourier transform of a correlation function. For spectra, we are often interested in such questions as:

- At what frequency is the spectrum a maximum?
- How rapidly does the intensity decrease as ω moves away from the location of the maximum?
- How rapidly does the spectrum go to zero as $\omega \to \infty$.

This leads us to ask the following related questions about Fourier transforms.

- Given a function $F(t)$, at which frequency is $\hat{F}(\omega)$ a maximum?
- How does $\hat{F}(\omega)$ change as ω moves away from the location of a maximum?
- What is the behavior of $\hat{F}(\omega)$ as $\omega \to \pm\infty$?

We will now discuss such questions.

Let us first consider functions of t that are real and nonnegative.

$$F(t) \geq 0 \quad \text{for all real } t$$

It is easy to show that the maximum in the absolute value of the Fourier transform occurs at $\omega = 0$.

$$|\hat{F}(\omega)| \;=\; \left|\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{i\omega t} F(t)\right| \leq \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, \left|e^{i\omega t}\right| |F(t)|$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega\, F(t) = \hat{F}(0)$$

Hence

$$|\hat{F}(\omega)| \le \hat{F}(0)$$

Exercise 5. Compare the predictions of this statement with the actual behavior of F_1, $\hat{F}_1$, F_2 and $\hat{F}_2$ of exercises 1 and 2.

Next let's discuss functions of t that are not only real and nonnegative but also have a single maximum and decay to zero on each side of the maximum. Such a function is often characterized by a half width at half height (HWHH). This is the half the interval between the times at which the function is half its maximum. The Fourier transform of such a function can also be characterized by its half width at half height.

For $F_1(t)$, for example, the function is half its maximum at $t = \pm(\ln 2)/b$. Thus the half width at half height is $(\ln 2)/b$ or $0.693b$. The HWHH of $\hat{F}_1(\omega)$ is equal to b. Note that for this case, the product of the HWHH of $F_1(t)$ and the HWHH of $\hat{F}_1(\omega)$ is 0.693, for all values of b.

Exercise 6. Consider the function

$$F_3(t) = Ae^{-bt^2}$$

What is the HWHH of this function? Calculate[3] $\hat{F}_3(\omega)$? What is the HWHH of the Fourier transform? What is the product of the two values of HWHH?

Exercise 7. Answer the questions of Exercise 6 for

$$\begin{aligned} F_4(t) &= A \quad \text{for } |t| < a \\ &= 0 \quad \text{for } |t| > a \end{aligned}$$

These results are examples of a very general principle: namely, if $F(t)$ is nonnegative and has a single maximum,

[3]Hint: complete the square.

- $\hat{F}(\omega)$ has a maximum at $\omega = 0$,
- the HWHH of $F(t)$ and of $\hat{F}(\omega)$ are inversely related, and
- their product is usually close to unity.

The next case to consider is that of a function of the form

$$F(t) = e^{-i\omega_0 t} f(t)$$

where $f(t)$ has the characteristics discussed in the paragraphs above; namely $f(t)$ is nonnegative and has a single maximum. Applying the fourth of the elementary properties discussed above, we immediately see that $\hat{F}(\omega)$ has a maximum at $\omega = \omega_0$. Moreover, its shape is identical to that of $\hat{f}(\omega)$, except that it has been shifted along the ω axis by an amount ω_0. In particular, it has the same HWHH as $\hat{f}(\omega)$.

Finally, let us consider a function of the form

$$F(t) = f(t) \cos \omega_0 t$$

where $f(t)$ is nonnegative and has a single maximum. We can rewrite this as

$$F(t) = \frac{1}{2} e^{i\omega_0 t} f(t) + \frac{1}{2} e^{-i\omega_0 t} f(t)$$

Applying the first and fourth elementary properties, we see that

$$\hat{F}(\omega) = \frac{1}{2}\left(\hat{f}(\omega + \omega_0) + \hat{f}(\omega - \omega_0)\right)$$

Thus, $\hat{F}(\omega)$ is a sum of two functions. One is peaked at $\omega = -\omega_0$ and the other is peaked at $\omega = \omega_0$. Each function has the same HWHH, that of $\hat{f}(\omega)$ itself. Thus, if ω_0 is large enough compared to this HWHH, $\hat{F}(\omega)$ has two distinguishable peaks. $F_2(t)$ in Exercise 2 is an example of such a function.

4 High frequency behavior of Fourier transforms

If $F(t)$ is a continuous (or piecewise continuous) function of time, $\hat{F}(\omega) \to 0$ as $\omega \to \pm\infty$. This statement is known as the Riemann-Lebesque lemma.

We will not prove it here, but it is important to understand the basis of the lemma, which we shall discuss.

Consider the special case that $F(t)$ is real. Thus the real part of $\hat{F}(\omega)$ is

$$\text{Re } \hat{F}(\omega) = \int_{-\infty}^{\infty} dt\, F(t) \cos \omega t$$

For large ω, the cosine function is a rapidly oscillatory function of time, and there will be extensive cancellation in the integration. This cancellation becomes more and more effective as $\omega \to \infty$ and so the integral approaches zero. A similar argument holds for the imaginary part of $\hat{F}(\omega)$, and it is easy to generalize these considerations to the case of complex $F(t)$.

The functions F_1, F_2, F_3, and F_4 in the exercises illustrate this theorem.

From the Riemann-Lebesque lemma, we expect that even though $\hat{F}(\omega)$ may be large for a certain range of ω, for large enough values of $|\omega|$ it will start to approach zero in some systematic way. How large does $|\omega|$ have to be before this systematic decay takes place and $\hat{F}(\omega)$ becomes small compared to its maximum value?

First consider the case in which $F(t)$ is continuous and differentiable, and suppose $F(t)$ and its first derivative are bounded. Then over any short enough time interval, $F(t)$ can be approximated as a straight line

$$F(t) \approx F(a) + F'(a)(t-a) \quad \text{for } a \leq t \leq b$$

Suppose $b - a$ is small enough that the maximum change in F over this interval, namely $F'(a)(b-a)$, is small compared with the maximum value of $F(t)$.

$$|F'(a)(b-a)| \leq |\text{Max } F(t)|$$

Next suppose that ω is large enough that $e^{i\omega t}$ oscillates many times during that interval, i.e.

$$|\omega|(b-a) >> 2\pi$$

Under these conditions, we expect substantial cancellation in this interval when $\hat{F}(\omega)$ is calculated because $F(t)$ is almost constant in the interval, and the cancellation becomes more and more extensive as $|\omega|$ is increased.

Combining these results together, we find the following approximate condition for extensive cancellation in the interval.

$$|\omega| >> \frac{2\pi}{b-a} >> \frac{2\pi|F'(a)|}{|\text{Max } F(t)|}$$

For cancellation in all intervals, we need

$$|\omega| >> \frac{2\pi|\text{Max } F'(a)|}{|\text{Max } F(t)|}$$

This illustrates a general principle that the large frequency behavior of $\hat{F}(\omega)$ is dominated by those intervals of t in which $F(t)$ is most rapidly varying[4], in this case the interval in which $|F'(t)|$ is largest.

This is only an approximate guide, but it can be very useful.

Exercise 8. Apply this criterion to the function F_1 of Exercise 1. Compare what it predicts to the actual behavior of the Fourier transform.

Exercise 9. Do the same thing for F_2 of Exercise 2.

We now want to consider the manner in which a Fourier transform approaches zero. We will state some principles without proof and give some examples. In general, as noted above, the large frequency behavior of $\hat{F}(\omega)$ is determined by the intervals in which $F(t)$ changes most rapidly.

Let us first consider a function with a jump discontinuity, which is in some sense the most rapid possible change for a function. As an example, consider

$$\begin{aligned} F_5(t) &= 0 \quad \text{for } t < 0 \\ &= Ae^{-bt} \quad \text{for } t > 0 \end{aligned}$$

[4]One sometimes hears the incorrect statement that "the large frequency behavior of $\hat{F}(\omega)$ is determined by the short time behavior of $F(t)$." The correct statement is the one given above.

This function jumps discontinuously from 0 to A at $t = 0$. The Fourier transform is eacily calculated to be

$$F_5(\omega) = \frac{iA}{\omega + ib}$$

which for large $|\omega|$ is iA/ω. This behavior is quite general. If a function $F(t)$ jumps discontinuously by an amount A at $t = 0$, its large $|\omega|$ dependence has a part that varies as

$$\hat{F}(\omega) \approx \frac{iA}{\omega}$$

This is a very slow decay.

Exercise 10. Consider the function

$$\begin{aligned} F_6(t) &= A_1 e^{b_1 t} \quad \text{for } t < 0 \\ &= A_2 e^{-b_2 t} \quad \text{for } t > 0 \end{aligned}$$

where $b_1, b_2 > 0$. This function has a jump of $A_1 - A_2$ at $t = 0$. Evaluate its Fourier tranform exactly and show that the large $|\omega|$ behavior is consistent with the statement above.

Exercise 11. Suppose a function jumps discontinuously by an amount A at $t = a$ rather than at $t = 0$. What is the large $|\omega|$ behavior of its Fourier transform?

If a function has several jump discontinuities, each discontinuity contributes additively to the behavior of the Fourier transform at large $|\omega|$.

Exercise 12. Consider the function F_4 in Exercise 7. Locate the jump discontinuities, and use the previous discussion to construct a formula for the large $|\omega|$ behavior of $\hat{F}_4(\omega)$.

Next, consider the case of a function that has no jump discontinuity but that does have a discontinuous first derivative. An example is $F_1(t)$ of Exercise 1. Its derivative jumps by an amount $-2bA$ at $t = 0$.

Exercise 13. Verify the previous statement.

For large $|\omega|$, $\hat{F}_1(\omega)$ is

$$\hat{F}_1(\omega) \approx -(-2bA)/\omega^2$$

In general, if a function has no jump discontinuities, but its first derivative has a jump of B at $t = 0$, the Fourier transform goes as $-B/\omega^2$ for large $|\omega|$.

Exercise 14. Consider the function

$$\begin{aligned} F_7(\omega) &= Ae^{b_1 t} \quad \text{for } t < 0 \\ &= Ae^{-b_2 t} \quad \text{for } t > 0 \end{aligned}$$

Evaluate its Fourier transform exactly, evaluate the jump in the derivative at $t = 0$, and verify that its large $|\omega|$ dependence is consistent with the principle stated above.

Exercise 15. Suppose a function is continuous and has a continuous derivative except that there is a jump discontinuity in the derivative at $t = a$. If the amount of the jump is B, what is the large $|\omega|$ behavior of the Fourier transform.

The same ideas can be extended to higher derivatives. If $F(t)$ and its first $n-$ 1 derivatives are continuous but the nth derivative has a jump discontinuity, the large $|\omega|$ dependence is $A\omega^{-(n+1)}$, where the amplitude A is related to the amount and location of the jump. If all derivatives of $F(t)$ exist, then, as $|\omega| \to \infty$, $\hat{F}(\omega)$ must go to zero more quickly than any inverse power of ω. (The previous sentence is very important. Read it again. Whenever, in the future, you are trying to understand the shape of spectral lines in the far wings, remember this statement.)

Answers.[5]

[5] Use these to check your results or to continue working if you get stuck.

1. $\hat{F}_1(\omega) = 2bA/(\omega^2 + b^2)$

2.

$$\hat{F}_2(\omega) = bA\left(\frac{1}{(\omega-\omega_0)^2+b^2} + \frac{1}{(\omega+\omega_0)^2+b^2}\right)$$

6. $\hat{F}_3(\omega) = A(\pi/b)^{1/2}e^{-\omega^2/4b}$

7.

$$\hat{F}_4(\omega) = 2Aa\frac{\sin\omega a}{\omega a}$$

12. The result you get by this analysis should be correct at large $|\omega|$. It turns out, however, that in this case the result is correct at all ω. This is an artifact of the particular simple form of F_4.