Each microstate with energy E has probability $1/g(E)$.

We will therefore perform a Metropolis Monte Carlo calculation using

$$p_\alpha = \frac{1}{g(E_\alpha)}$$

where E_α is the energy associated with microstate α.

Hence, $p_{\alpha\beta} = \pi_{\alpha\beta} \min\left(1, \frac{g(E_\alpha)}{g(E_\beta)}\right)$

<u>But, we do not know $g(E)$!</u>

We need to construct it as we go along.

Here is how:

Construct a histogram $\underline{H(E)}$

and the density of states $g(E)$.

Start by setting $H(E) = 0$ and

$g(E) = 1$.

Define a factor $f = e \; (= 2.718281828\ldots)$.

Start performing the Markov process using the Metropolis rule

$$p_{\alpha\beta} = \pi_{\alpha\beta} \min\left(1, \frac{g(E_\alpha)}{g(E_\beta)}\right).$$

For each visited state α, <u>accepted or not</u> update

$$H(E_\alpha) \to H(E_\alpha) + 1$$

$$g(E_\alpha) \to f \cdot g(E_\alpha)$$

Continue until the histogram is "sufficiently" flat.

Then reset the histogram to zero and let $f \to \sqrt{f}$.

Repeat procedure until $\ln f \simeq 10^{-8}$.

Wang and Landau comment in

Phys. Rev. Lett. 86, 2050 (2001):

"Our algorithm is based on the observation that if we perform a random walk in energy space with a probability proportional to the reciprocal of the density of states, $1/g(E)$, then a flat histogram for the energy distribution is generated."

Spectral Methods

The Fourier transform:

$$h(t) \rightleftarrows H(f)$$

time domain — frequency domain

$$\begin{cases} H(f) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{+\infty} dt \; h(t)\, e^{2\pi i f t} \\ h(t) = \dfrac{1}{\sqrt{2\pi}} \displaystyle\int_{-\infty}^{+\infty} df \; H(f)\, e^{-2\pi i f t} \end{cases}$$

Some properties:

$h(t)$	$H(f)$
$h(at)$	$\frac{1}{\lvert a\rvert} H\left(\frac{f}{\lvert a\rvert}\right)$
$h(t-t_0)$	$H(f)\, e^{2\pi i f t_0}$

Convolution:

$$(g * h)(t) = \int_{-\infty}^{+\infty} d\tau \, g(\tau) \, h(t-\tau)$$

$$G(f) H(f)$$

Correlation

$$\langle g \, h \rangle (t) = \int_{-\infty}^{+\infty} d\tau \, g(t+\tau) \, h(\tau)$$

$$G(f) H^{*}(f).$$

Wiener - Khinchin theorem:

$$\langle g^2 \rangle (t) \qquad\qquad | G(f) |^2$$

Parseval theorem:

$$\int_{-\infty}^{+\infty} dt \, | h(t) |^2 = \int_{-\infty}^{+\infty} df \, | H(f) |^2$$

The power spectrum:

Two-sided power spectrum:

$$P_h(f) = |H(f)|^2$$

One-sided power spectrum:

$$P_h(f) = |H(f)|^2 + |H(-f)|^2$$

Total power (Parseval theorem):

$$\int_{-\infty}^{+\infty} P_h(f)\,df = \int_{-\infty}^{+\infty} |h(t)|^2\,dt$$

two-sided
power spectrum

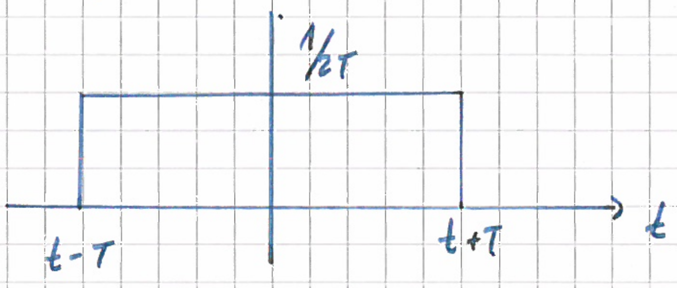
Problem if $|h(t)|^2$ does not approach zero fast enough for $t \to \pm\infty$. ...

ensure convergence of the integral.

We then need to define the <u>power spectral density per time unit.</u>

To do this, we define a window

$$h(t) \to \underbrace{\frac{1}{2T}\,\theta(t+T)\,\theta(T-t)}\,h(t)$$



$$H(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} h(t)\, e^{2\pi i f t}\, dt$$

$$\to \frac{1}{2T}\,\frac{1}{\sqrt{2\pi}} \int_{-T}^{+T} h(t)\, e^{2\pi i f t}\, dt .$$

The Parseval theorem:

$$\int_{-\infty}^{+\infty} df\, |H(f)|^2 = \frac{1}{2\pi} \int_{-\infty}^{+\infty} df \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\, h(t)\, h^*(t')\, e^{2\pi i f (t-t')}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\, h(t)\, h^*(t') \underbrace{\int_{-\infty}^{+\infty} df\, e^{2\pi i f (t-t')}}_{2\pi\, \delta(t-t')}$$

$$= \int_{-\infty}^{+\infty} dt \int_{-\infty}^{+\infty} dt'\, h(t)\, h^*(t')\, \delta(t-t')$$

$$= \int_{-\infty}^{+\infty} dt\, |h(t)|^2$$

When integrating only on the interval

$t \in [-T, T]$:

$$2T \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} df\, H(f)\, e^{-2\pi i f t}$$

$$= 2T \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} df \, e^{-2\pi i f t} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dt'$$

$$\underbrace{\frac{1}{2T} \theta(t'+T)\,\theta(T-t')}\, h(t')\, e^{2\pi i f t'}$$

Using the window:

$$= \int_{-T}^{T} dt' \, h(t') \; \frac{1}{2\pi} \int_{-\infty}^{+\infty} df \, e^{2\pi i f (t'-t)}$$

$$= \int_{-T}^{T} dt' \, h(t') \, \delta(t'-t) = \begin{cases} 0 & \text{if } t < -T \\ h(t) & \text{if } -T < t < T \\ 0 & \text{if } t > T. \end{cases}$$

Hence, we identify

$$\int_{-\infty}^{+\infty} df \rightarrow 2T \int_{-\infty}^{+\infty} df$$

Implementing the window.

$$\boxed{2T \int_{-\infty}^{+\infty} df \, |H(f)|^2 = \frac{1}{2T} \int_{-T}^{T} dt \, |h(t)|^2}$$

Parseval on a window.

Discrete data sampling

$$t = n\Delta \quad ; \quad n \in \mathbb{Z}$$

$$h(t) \to h_n = h(n\Delta)$$

This is the sampling interval.

$$\boxed{\text{Sampling interval} = 1/\text{sampling rate.}}$$

Sampling rate = # samplings per unit time interval.

The Nyquist critical frequency:

$$\boxed{f_c = \frac{1}{2\Delta}}$$

Assume $h(t)$ continuous and <u>band width limited.</u>

That is, $H(f) = 0$ for all $|f| \geq f_c$.

Then $h(t)$ is completely determined by h_n:

$$\boxed{h(t) = \Delta \sum_{n=-\infty}^{+\infty}{}' h_n \frac{\sin 2\pi f_c (t - n\Delta)}{\pi (t - n\Delta)}}$$

<u>This is the sampling theorem.</u>

<u>Example</u>: $h(t) = \sin t = \frac{1}{2i}(e^{it} - e^{-it})$

$$\underline{H(f)} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dt\, e^{2\pi i f t} \frac{1}{2i}(e^{it} - e^{-it})$$

$$\underline{= \sqrt{\frac{\pi}{2}} \frac{1}{i} \left\{ \delta(1 + 2\pi f) - \delta(1 - 2\pi f) \right\}}$$

Hence $H(f) \neq 0$ for $f = \pm \frac{1}{2\pi}$

If we now set the sampling interval at π, this is $\frac{1}{2f}$ when $f = \frac{1}{2\pi}$.

We measure $h(t)$ at intervals π:

$$\underline{h_n = \sin(\delta + n\pi)}.$$

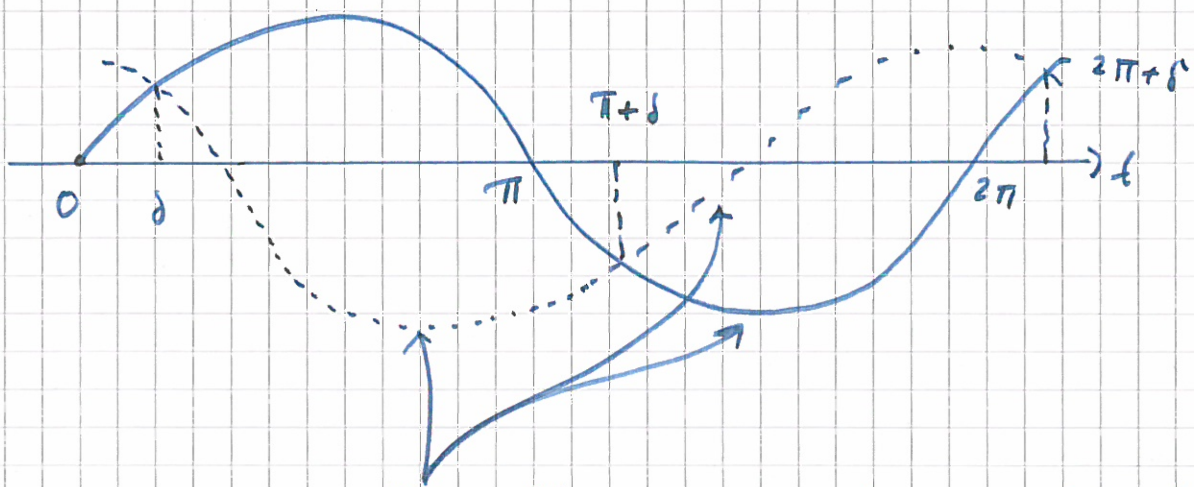
The sampling theorem gives

$$\underline{\pi \sum_{n=-\infty}^{+\infty}{}' \sin(\delta + n\pi) \frac{\sin(t - n\pi)}{\pi(t - n\pi)}}$$

$$= \sum_{n=-\infty}^{+\infty}{}' (-1)^n \sin\delta \frac{(-1)^n \sin t}{(t - n\pi)}$$

$$= \sin\delta \sin t \underbrace{\sum_{n=-\infty}^{+\infty}{}' \frac{1}{t - n\pi}}_{\cot t} = \underline{\sin\delta \cot t}.$$

This is not what we started with and something has gone wrong.



At this sampling rate, the reconstruction is <u>not</u> unique.

(This is <u>aliasing</u> as we will come to.)

Rather, we sample at (e.g.) a ~~rate~~ interval $\pi/2$.

Let us also for simplicity sample at $\delta = 0$: $\underline{h_n = \sin \frac{\pi}{2} n.}$

We then have

$$\Delta \sum_{n=-\infty}^{+\infty}{}' \sin n\Delta \; \frac{\sin \frac{\pi}{\Delta}(t-n\Delta)}{\pi(t-n\Delta)}$$

$$= \sum_{n=-\infty}^{+\infty}{}' \sin\left(n\frac{\pi}{2}\right) \frac{\sin(2t-n\pi)}{2\left(t-n\frac{\pi}{2}\right)}$$

$$= \sum_{n=-\infty}^{+\infty}{}' (-1)^n \sin\left(n\frac{\pi}{2}\right) \frac{\sin 2t}{2t-n\pi}$$

$$= (-1) \sum_{n=-\infty}^{+\infty}{}' (-1)^n \frac{\sin 2t}{2t-2n\pi-\pi}$$

$$= -\sin 2t \sum_{n=-\infty}^{+\infty}{}' \frac{(-1)^n}{2\left(t-\frac{\pi}{2}\right)-2n\pi}$$

$$= -\sin t \cos t \left[\underbrace{\frac{1}{t-\frac{\pi}{2}} + \sum_{n=1}^{\infty}{}' \frac{(-1)^n \, 2\left(t-\frac{\pi}{2}\right)}{\left(t-\frac{\pi}{2}\right)^2 - n^2\pi^2}}_{=\frac{1}{\sin\left(t-\frac{\pi}{2}\right)}} \right]$$

$$\underline{= \sin t}$$

A serious problem: <u>Aliasing</u>

(See J. Fondi, EJP <u>28</u>, 551 (2007)).

Aliasing occurs when $f_c = \frac{1}{2\Delta}$ is smaller than the band width (1.2) of the signal.

A familiar example: Cart wheels that seems to rotate backwards when filmed.

Fourier sampling: Two frequencies f_1 and f_2 are related as

$$f_2 = f_1 + \frac{k}{\Delta}.$$

Then $\underline{e^{2\pi i f_2 \overset{t}{\widetilde{n\Delta}}}} = e^{2\pi i (f_1 + \frac{k}{\Delta}) n\Delta}$

$$= e^{2\pi i f_1 n\Delta} e^{2\pi i k n} = \underline{e^{2\pi i f_1 n\Delta}}.$$

As long as $h(t)$ is band width limited and sampling rate is sufficiently large so that

$$H(f) \to 0 \text{ as } |f| \to f_c,$$

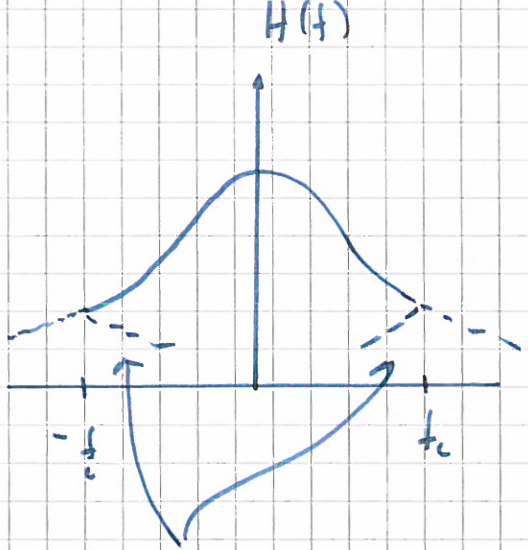
there will be no aliasing since

$$\text{if} \quad -f_c < f_1 < f_c \Rightarrow$$

$$f_2 = f_1 + \frac{k}{\Delta} = f_1 + 2f_c k > f_c$$

or

$$f_2 < -f_c .$$



folded back into signal ⇒ aliasing.

(2) Filter continuous signal to produce a new signal with finite and known band width. Choose Δ accordingly.

Discrete Fourier transforms

Discretizing signal:

$$h_k = h(k\Delta), \quad k = \underbrace{0, \dots, N-1}$$

N sampling points

even number.

With N sampling points, we cannot produce more than N Fourier transforms: N frequencies.

We choose the N+1 frequencies

$$f_n = \frac{n}{N\Delta},$$

$$n = -\frac{N}{2}, \dots, \frac{N}{2}.$$

As will be evident later on,

$$H(f_c) = H\left(\frac{1}{2\Delta}\right) = H(-f_c)$$

Nyquist frequency.

$$\left(n = \pm \frac{N}{2}\right)$$

Thus, there are only
N independent $H(f_n)$.

We approximate the Fourier integral
by a sum:

$$H(f_n) = \cancel{\frac{1}{\sqrt{2\pi}}} \int_{-\infty}^{+\infty} h(t)\, e^{2\pi i f_n t}\, dt$$

We drop this

$$= \Delta \sum_{k=0}^{N-1} h_k\, e^{2\pi i f_n t_k}$$

$$= \Delta \sum_{k=0}^{N-1} h_k \, e^{2\pi i k n / N}$$

We define

$$\boxed{H_n = \sum_{k=0}^{N-1} h_k \, e^{2\pi i k n / N}}$$

At the Nyquist frequency, f_c:

$$\underline{H_{-\frac{N}{2}}} = \sum_{k=0}^{N-1} h_k \, e^{2\pi i \left(-\frac{N}{2}\right)\frac{1}{N} k}$$

$$= \sum_{k=0}^{N-1} h_k \, e^{2\pi i \left(-\frac{N}{2}\right)\frac{k}{N}} \, e^{2\pi i k \frac{N}{N}}$$

$$= \sum_{k=0}^{N-1} h_k \, e^{2\pi i \left(+\frac{N}{2}\right)\frac{k}{N}} = \underline{H_{+\frac{N}{2}}}$$

In general:

$$\boxed{H_{-n} = H_{N-n}}$$

Usually, negative frequencies are avoided.

$$f = 0 \Rightarrow n = 0$$

$$0 < f < f_c \Rightarrow 1 \leq n \leq \frac{N}{2} - 1$$

$$-f_c < f < 0 \Rightarrow \frac{N}{2} + 1 \leq n \leq N - 1$$

$$\left.\begin{array}{l} f = f_c \\ f = -f_c \end{array}\right\} \Rightarrow n = \frac{N}{2}.$$

Discrete inverse Fourier transform:

$$\boxed{h_k = \frac{1}{N} \sum_{n=0}^{N-1} H_n \, e^{-2\pi i k n/N}}$$

By the shift in frequencies, using the symmetry $H_{-n} = H_{N-n}$, we now have the same range of n to sweep over as in the direct Fourier transform.

Discrete version of Parseval theorem:

$$\boxed{\sum_{k=0}^{N-1} |h_k|^2 = \frac{1}{N} \sum_{n=0}^{N-1} |H_n|^2}$$