

Thermal cantilever calibration

Equipartition theorem and power spectral density fitting

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1 Overview

In order to measure forces accurately with an Atomic Force Microscope (AFM), it is important to measure the cantilever spring constant. The force exerted on the cantilever can then be deduced from it's deflection via Hooke's law $F = -kx$.

The basic idea is to use the equipartition theorem[1],

$$\frac{1}{2}k\langle x^2 \rangle = \frac{1}{2}k_B T, \quad (1)$$

where k_B is Boltzmann's constant, T is the absolute temperature, and $\langle x^2 \rangle$ denotes the expectation value of x^2 as measured over a very long interval t_T ,

$$\langle A \rangle \equiv \lim_{t_T \rightarrow \infty} \frac{1}{t_T} \int_{-t_T/2}^{t_T/2} A dt. \quad (2)$$

Solving the equipartition theorem for k yields

$$k = \frac{k_B T}{\langle x^2 \rangle}, \quad (3)$$

so we need to measure (or estimate) the temperature T and variance of the cantilever position $\langle x^2 \rangle$ in order to estimate k .

1.1 Related papers

Various corrections taking into account higher order modes [2, 8], and cantilever tilt [9] have been proposed and reviewed [5, 6, 7], but we will focus here on the derivation of Lorentzian noise in damped simple harmonic oscillators that underlies all frequency-space methods for improving the basic $k\langle x^2 \rangle = k_B T$ method.

Roters and Johannsmann describe a similar approach to deriving the Lorentzian power spectral density[3].

WARNING: It is popular to refer to the power spectral density as a ‘‘Lorentzian’’[1, 3, 6, 5] even though eq. 53 differs from the classic Lorentzian[4].

$$L(x) = \frac{1}{\pi} \frac{\frac{1}{2}\Gamma}{(x - x_0)^2 + (\frac{1}{2}\Gamma)^2} \quad (4)$$

It is unclear whether the references are due to uncertainty about the definition of the Lorentzian or to the fact that eq. 53 is also peaked. In order to avoid any uncertainty, we will leave eq. 53 unnamed.

2 Methods

To find $\langle x^2 \rangle$, the raw photodiode voltages $V_p(t)$ are converted to distances $x(t)$ using the photodiode sensitivity σ_p (the slope of the voltage vs. distance curve of data taken while the tip is in contact with the surface) via

$$x(t) = \frac{V_p(t)}{\sigma_p} \quad (5)$$

Rather than computing the variance of $x(t)$ directly, we attempt to filter out noise by fitting the spectral power density (PSD) of $x(t)$ to the theoretically predicted PSD for a damped harmonic oscillator (eq. 53)

$$\ddot{x} + \beta\dot{x} + \omega_0^2 x = \frac{F_{\text{thermal}}}{m} \quad (6)$$

$$\text{PSD}(x, \omega) = \frac{G_1}{(\omega_0^2 - \omega^2)^2 + \beta^2 \omega^2}, \quad (7)$$

where $G_1 \equiv G_0/m^2$, ω_0 , and β are used as the fitting parameters (see eqn.s 53). The variance of $x(t)$ is then given by eq. 59

$$\langle x(t)^2 \rangle = \frac{\pi G_1}{2\beta\omega_0^2}, \quad (8)$$

which we can plug into the equipartition theorem (eqn. 1) yielding

$$k = \frac{2\beta\omega_0^2 k_B T}{\pi G_1}. \quad (9)$$

From eqn. 61, we find the expected value of G_1 to be

$$G_1 \equiv G_0/m^2 = \frac{2}{\pi m} k_B T \beta. \quad (10)$$

2.1 Fitting deflection voltage directly

In order to keep our errors in measuring σ_p separate from other errors in measuring $\langle x(t)^2 \rangle$, we can fit the voltage spectrum before converting to distance.

$$\ddot{V}_p/\sigma_p + \beta\dot{V}_p/\sigma_p + \omega_0^2 V_p/\sigma_p = F_{\text{thermal}} \quad (11)$$

$$\ddot{V}_p + \beta\dot{V}_p + \omega_0^2 V_p = \sigma_p \frac{F_{\text{thermal}}}{m} \quad (12)$$

$$\ddot{V}_p + \beta\dot{V}_p + \omega_0^2 V_p = \frac{F_{\text{thermal}}}{m_p} \quad (13)$$

$$\text{PSD}(V_p, \omega) = \frac{G_{1p}}{(\omega_0^2 - \omega^2)^2 + \beta^2 \omega^2} \quad (14)$$

$$\langle V_p(t)^2 \rangle = \frac{\pi G_{1p}}{2\beta\omega_0^2} = \frac{\pi\sigma_p^2 G_1}{2\beta\omega_0^2} = \sigma_p^2 \langle x(t)^2 \rangle, \quad (15)$$

where $m_p \equiv m/\sigma_p$, $G_{1p} \equiv G_0/m_p^2 = \sigma_p^2 G_1$. Plugging into the equipartition theorem yields

$$k = \frac{\sigma_p^2 k_B T}{\langle V_p(t)^2 \rangle} = \frac{2\beta\omega_0^2 \sigma_p^2 k_B T}{\pi G_{1p}}. \quad (16)$$

From eqn. 10, we find the expected value of G_{1p} to be

$$G_{1p} \equiv \sigma_p^2 G_1 = \frac{2}{\pi m} \sigma_p^2 k_B T \beta. \quad (17)$$

2.2 Fitting deflection voltage in frequency space

Note: the math in this section depends on some definitions from section 3.

As yet another alternative, you could fit in frequency $f \equiv \omega/2\pi$ instead of angular frequency ω . But we must be careful with normalization. Comparing the angular frequency and normal frequency unitary Fourier transforms

$$\mathcal{F}\{x(t)\}(\omega) \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x(t) e^{-i\omega t} dt \quad (18)$$

$$\mathcal{F}_f\{x(t)\}(f) \equiv \int_{-\infty}^{\infty} x(t) e^{-2\pi i f t} dt = \int_{-\infty}^{\infty} x(t) e^{-i\omega t} dt = \sqrt{2\pi} \cdot \mathcal{F}\{x(t)\}(\omega = 2\pi f), \quad (19)$$

from which we can translate the PSD

$$\text{PSD}(x, \omega) \equiv \lim_{t_T \rightarrow \infty} \frac{1}{t_T} 2 |\mathcal{F}\{x(t)\}(\omega)|^2 \quad (20)$$

$$\text{PSD}_f(x, f) \equiv \lim_{t_T \rightarrow \infty} \frac{1}{t_T} 2 |\mathcal{F}_f\{x(t)\}(f)|^2 = 2\pi \cdot \lim_{t_T \rightarrow \infty} \frac{1}{t_T} 2 |\mathcal{F}\{x(t)\}(\omega = 2\pi f)|^2 = 2\pi \text{PSD}(x, \omega = 2\pi f). \quad (21)$$

The variance of the function $x(t)$ is then given by plugging into eqn. 34 (our corollary to Parseval's theorem)

$$\langle x(t)^2 \rangle = \int_0^\infty \text{PSD}(x, \omega) d\omega = \int_0^\infty \frac{1}{2\pi} \text{PSD}_f(x, f) 2\pi \cdot df = \int_0^\infty \text{PSD}_f(x, f) df. \quad (22)$$

Therefore

$$\text{PSD}_f(V_p, f) = 2\pi \text{PSD}(V_p, \omega) = \frac{2\pi G_{1p}}{(4\pi f_0^2 - 4\pi^2 f^2)^2 + \beta^2 4\pi^2 f^2} = \frac{2\pi G_{1p}}{16\pi^4 (f_0^2 - f^2)^2 + \beta^2 4\pi^2 f^2} = \frac{G_{1p}/8\pi^3}{(f_0^2 - f^2)^2 + \frac{\beta^2 f^2}{4\pi^2}} \quad (23)$$

$$= \frac{G_{1f}}{(f_0^2 - f^2)^2 + \beta_f^2 f^2} \quad (24)$$

$$\langle V_p(t)^2 \rangle = \frac{\pi G_{1f}}{2\beta_f f_0^2}. \quad (25)$$

where $f_0 \equiv \omega_0/2\pi$, $\beta_f \equiv \beta/2\pi$, and $G_{1f} \equiv G_{1p}/8\pi^3$. Finally

$$k = \frac{\sigma_p^2 k_B T}{\langle V_p(t)^2 \rangle} = \frac{2\beta_f f_0^2 \sigma_p^2 k_B T}{\pi G_{1f}}. \quad (26)$$

From eqn. 10, we expect G_{1f} to be

$$G_{1f} = \frac{G_{1p}}{8\pi^3} = \frac{\sigma_p^2 G_1}{8\pi^3} = \frac{2}{\pi m} \frac{\sigma_p^2 k_B T \beta}{8\pi^3} = \frac{\sigma_p^2 k_B T \beta}{4\pi^4 m}. \quad (27)$$

3 Theoretical power spectral density for a damped harmonic oscillator

Our cantilever can be approximated as a damped harmonic oscillator

$$m\ddot{x} + \gamma\dot{x} + kx = F(t), \quad (28)$$

where x is the displacement from equilibrium, m is the effective mass, γ is the effective drag coefficient, k is the spring constant, and $F(t)$ is the external driving force. During the non-contact phase of calibration, $F(t)$ comes from random thermal noise.

In the following analysis, we use the unitary, angular frequency Fourier transform normalization

$$\mathcal{F}\{x(t)\} \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x(t) e^{-i\omega t} dt \quad (29)$$

We also use the following theorems (proved elsewhere):

$$\cos\left(\frac{\theta}{2}\right) = \pm \sqrt{\frac{1}{2}[1 + \cos(\theta)]} \quad [10], \quad (30)$$

$$\mathcal{F}\left\{\frac{d^n x(t)}{dt^n}\right\} = (i\omega)^n x(\omega) \quad [11], \quad (31)$$

$$\int_{-\infty}^{\infty} |x(t)|^2 dt = \int_{-\infty}^{\infty} |x(\omega)|^2 d\omega \quad (\text{Parseval's}) [12]. \quad (32)$$

As a corollary to Parseval's theorem, we note that the one sided power spectral density per unit time (PSD) defined by

$$\text{PSD}(x, \omega) \equiv \lim_{t_T \rightarrow \infty} \frac{1}{t_T} 2|x(\omega)|^2 \quad [13] \quad (33)$$

relates to the variance by

$$\langle x(t)^2 \rangle = \lim_{t_T \rightarrow \infty} \frac{1}{t_T} \int_{-t_T/2}^{t_T/2} |x(t)|^2 dt = \lim_{t_T \rightarrow \infty} \frac{1}{t_T} \int_{-\infty}^{\infty} |x(\omega)|^2 d\omega = \int_0^\infty \text{PSD}(x, \omega) d\omega, \quad (34)$$

where t_T is the total time over which data has been acquired.

We also use the Wiener-Khinchin theorem, which relates the two sided power spectral density $S_{xx}(\omega)$ to the autocorrelation function $r_{xx}(t)$ via

$$S_{xx}(\omega) = \mathcal{F} \{r_{xx}(t)\} \quad (\text{Wiener-Khinchin})[14], \quad (35)$$

where $r_{xx}(t)$ is defined in terms of the expectation value

$$r_{xx}(t) \equiv \langle x(\tau)\bar{x}(\tau-t) \rangle \quad [15] \quad (36)$$

and \bar{x} represents the complex conjugate of x .

3.1 Highly damped case

For highly damped systems, the inertial term becomes insignificant ($m \rightarrow 0$). This model is commonly used for optically trapped beads. Because it is simpler and solutions are more easily available, we'll use it outline the general approach before diving into the general case.

Fourier transforming eq. 28 with $m = 0$ and applying 31 we have

$$(i\gamma\omega + k)x(\omega) = F(\omega) \quad (37)$$

$$|x(\omega)|^2 = \frac{|F(\omega)|^2}{k^2 + \gamma^2\omega^2}. \quad (38)$$

We compute the PSD by plugging eq. 38 into 33

$$\text{PSD}(x, \omega) = \lim_{t_T \rightarrow \infty} \frac{1}{t_T} \frac{2|F(\omega)|^2}{k^2 + \gamma^2\omega^2}. \quad (39)$$

Because thermal noise is white (not autocorrelated + Wiener-Khinchin Theorem), we can denote the one sided thermal power spectral density per unit time by

$$\text{PSD}(F, \omega) = G_0 = \lim_{t_T \rightarrow \infty} \frac{1}{t_T} 2|F(\omega)|^2 \quad (40)$$

Plugging eq. 40 into 39 we have

$$\text{PSD}(x, \omega) = \frac{G_0}{k^2 + \gamma^2\omega^2}. \quad (41)$$

This is the formula we would use to fit our measured PSD, but let us go a bit farther to find the expected PSD and thermal noise given m , γ and k .

Integrating over positive ω to find the total power per unit time yields

$$\int_0^\infty \text{PSD}(x, \omega) d\omega = \int_0^\infty \frac{G_0}{k^2 + \gamma^2\omega^2} d\omega \quad (42)$$

$$= \frac{G_0}{\gamma} \int_0^\infty \frac{1}{k^2 + z^2} dz \quad (43)$$

$$= \frac{G_0\pi}{2\gamma k}, \quad (44)$$

where the integral is solved in Section 5.

Plugging into our corollary to Parseval's theorem (eq. 34),

$$\langle x(t)^2 \rangle = \frac{G_0\pi}{2\gamma k} \quad (45)$$

Plugging eq. 45 into eqn. 1 we have

$$k \frac{G_0\pi}{2\gamma k} = k_B T \quad (46)$$

$$G_0 = \frac{2\gamma k_B T}{\pi}. \quad (47)$$

So we expect $X(t)$ to have a power spectral density per unit time given by

$$\text{PSD}(x, \omega) = \frac{2}{\pi} \cdot \frac{\gamma k_B T}{k^2 + \gamma^2\omega^2}. \quad (48)$$

3.2 General form

The procedure here is exactly the same as the previous section. The integral normalizing G_0 just become a little more complicated...

Fourier transforming eq. 28 and applying 31 we have

$$(-m\omega^2 + i\gamma\omega + k)x(\omega) = F(\omega) \quad (49)$$

$$(\omega_0^2 - \omega^2 + i\beta\omega)x(\omega) = \frac{F(\omega)}{m} \quad (50)$$

$$|x(\omega)|^2 = \frac{|F(\omega)|^2/m^2}{(\omega_0^2 - \omega^2)^2 + \beta^2\omega^2}, \quad (51)$$

where $\omega_0 \equiv \sqrt{k/m}$ is the resonant angular frequency and $\beta \equiv \gamma/m$ is the drag-acceleration coefficient.

We compute the PSD by plugging eq. 51 into 33

$$\text{PSD}(x, \omega) = \lim_{t_r \rightarrow -\infty} \frac{1}{t_T} \frac{2|F(\omega)|^2/m^2}{(\omega_0^2 - \omega^2)^2 + \beta^2\omega^2}. \quad (52)$$

Plugging eq. 40 into 52 we have

$$\text{PSD}(x, \omega) = \frac{G_0/m^2}{(\omega_0^2 - \omega^2)^2 + \beta^2\omega^2}. \quad (53)$$

Integrating over positive ω to find the total power per unit time yields

$$\int_0^\infty \text{PSD}(x, \omega) d\omega = \frac{G_0}{2m^2} \int_{-\infty}^\infty \frac{1}{(\omega_0^2 - \omega^2)^2 + \beta^2\omega^2} d\omega \quad (54)$$

$$= \frac{G_0}{2m^2} \cdot \frac{\pi}{\beta\omega_0^2} \quad (55)$$

$$= \frac{G_0\pi}{2m^2\beta\omega_0^2} \quad (56)$$

$$= \frac{G_0\pi}{2m^2\beta\frac{k}{m}} \quad (57)$$

$$= \frac{G_0\pi}{2m\beta k} \quad (58)$$

The integration is detailed in Section 5. By our corollary to Parseval's theorem (eq. 34), we have

$$\langle x(t)^2 \rangle = \frac{G_0\pi}{2m^2\beta\omega_0^2} \quad (59)$$

Plugging eq. 59 into the equipartition theorem (eqn. 1) we have

$$k \frac{G_0\pi}{2m\beta k} = k_B T \quad (60)$$

$$G_0 = \frac{2}{\pi} k_B T m \beta. \quad (61)$$

So we expect $x(t)$ to have a power spectral density per unit time given by

$$\text{PSD}(x, \omega) = \frac{2k_B T \beta}{\pi m [(\omega_0^2 - \omega^2)^2 + \beta^2\omega^2]} \quad (62)$$

4 Contour integration

As a brief review, some definite integrals from $-\infty$ to ∞ can be evaluated by integrating along the contour C shown in Figure 1.

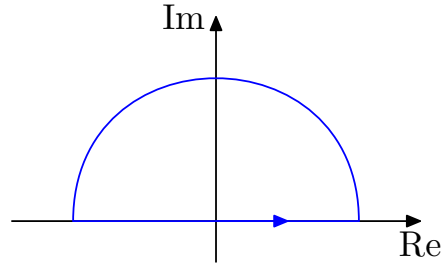


Figure 1: Integral contour C enclosing the upper half plane.

A sufficient condition on the function $f(z)$ to be integrated, is that $\lim_{|z| \rightarrow \infty} |f(z)|$ falls off at least as fast as $\frac{1}{z^2}$. When this is the case, the integral around the outer semicircle of C is 0, so the $\int_C f(z) dz = \int_{-\infty}^{\infty} f(z) dz$.

We can evaluate the integral using residue theorem

$$\int_C f(z) dz = \sum_{z_p \in \text{poles in } C} 2\pi i \text{Res}(z = z_p, f(z)), \quad (63)$$

where for simple poles (single roots)

$$\text{Res}(z = z_p, f(z)) = \lim_{z \rightarrow z_p} (z - z_p) f(z), \quad (64)$$

and in general for a pole of order n

$$\text{Res}(z = z_p, f(z)) = \frac{1}{(n-1)!} \cdot \lim_{z \rightarrow z_p} \frac{d^{n-1}}{dz^{n-1}} [(z - z_p)^n \cdot f(z)] \quad (65)$$

5 Integrals

5.1 Highly damped integral

$$I = \int_0^{\infty} \frac{1}{k^2 + z^2} dz \quad (66)$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \frac{1}{k^2 + z^2} dz \quad (67)$$

$$= \frac{1}{2k} \int_{-\infty}^{\infty} \frac{1}{u^2 + 1} du \quad (68)$$

$$(69)$$

where $u \equiv z/k$, $du = dz/k$. There are simple poles at $u = \pm i$

$$I = \frac{1}{2k} \cdot 2\pi i \text{Res}(z = i, f(u)) \quad (70)$$

$$= \frac{1}{2k} \cdot \frac{2\pi i}{i + i} \quad (71)$$

$$= \frac{1}{2k} \pi \quad (72)$$

$$= \frac{\pi}{2k}, \quad (73)$$

5.2 General case integral

We will show that for any $(a, b > 0) \in \mathbb{R}$

$$I = \int_{-\infty}^{\infty} \frac{1}{(a^2 - z^2) + b^2 z^2} dz = \frac{\pi}{ba^2}. \quad (74)$$

First we note that $|f(z)| \rightarrow 0$ like $|z|^{-4}$ for $|z| \gg 1$, and that $f(z)$ is even, so

$$I = \int_C \frac{1}{(a^2 - z^2)^2 + b^2 z^2} dz, \quad (75)$$

where C is the contour shown in Figure 1.

Because the denominator is of the form $A^2 + B^2$, we can factor it into $(A + iB)(A - iB)$ like so

$$(a^2 - z^2)^2 + b^2 z^2 = (a^2 - z^2 + ibz)(a^2 - z^2 - ibz) \quad (76)$$

And the roots of $z^2 \pm ibz - a^2$

$$z_{r\pm} = \pm \frac{ib}{2} \left(1 \pm \sqrt{1 - 4 \frac{-a^2}{(ib)^2}} \right) \quad (77)$$

$$= \pm \frac{ib}{2} \left(1 \pm \sqrt{1 - 4 \frac{a^2}{b^2}} \right) \quad (78)$$

$$= \pm \frac{ib}{2} (1 \pm S) \quad (79)$$

Where $S \equiv \sqrt{1 - 4 \frac{a^2}{b^2}}$.

To determine the nature and locations of the roots, consider the following cases (in order of increasing a).

- $a < b/2$, overdamped.
- $a = b/2$, critically damped.
- $a > b/2$, underdamped.

In the overdamped case $S \in \mathbb{R}$ and $S > 0$, so $z_{r\pm}$ is purely imaginary, and $z_{r+} = -z_{r-}$. For any $a < b/2$, we have $0 < S < 1$, so $\text{Im}(z_{r\pm}) > 0$. Thus, there are two single poles in the upper half plane ($z_{r\pm}$), and two single poles in the lower half plane ($-z_{r\pm}$).

In the critically damped case $S = 0$, so $z_{r+} = z_{r-}$, and we have double poles at $\pm z_{r+} = \pm \frac{ib}{2}$.

In the underdamped case S is purely imaginary, so $z_{r\pm}$ is complex, with z_{r+} in the 2nd quarter, and z_{r-} in the 1st quarter. The other two simple poles, $-z_{r-}$ and $-z_{r+}$, are in the 3rd and 4th quarters respectively.

Our contour C always encloses the poles $z_{r\pm}$. We will deal with the simple pole cases first, and then return to the critically damped case.

5.2.1 Over- and under-damped

Our factored function $f(z)$ is

$$f(z) = \frac{1}{(z - z_{r+})(z + z_{r+})(z + z_{r-})(z - z_{r-})} \quad (80)$$

Applying eq. 63 and 64 we have

$$I = 2\pi i (\text{Res}(z = z_{r+}, f(z)) + \text{Res}(z = z_{r-}, f(z))) \quad (81)$$

$$= 2\pi i \left(\frac{1}{(z_{r+} + z_{r+})(z_{r+} + z_{r-})(z_{r+} - z_{r-})} + \frac{1}{(z_{r-} - z_{r+})(z_{r-} + z_{r+})(z_{r-} + z_{r-})} \right) \quad (82)$$

$$= \frac{\pi i}{z_{r+}^2 - z_{r-}^2} \left(\frac{1}{z_{r+}} - \frac{1}{z_{r-}} \right) \quad (83)$$

$$= \frac{\pi i}{\left(\frac{ib}{2}(1+S)\right)^2 - \left(\frac{ib}{2}(1-S)\right)^2} \cdot \frac{z_{r-} - z_{r+}}{z_{r+}z_{r-}} \quad (84)$$

$$= \frac{-4\pi i/b^2}{(1+2S+S^2) - (1-2S+S^2)} \cdot \frac{\frac{ib}{2}[(1-S) - (1+S)]}{\left(\frac{ib}{2}\right)^2 (1+S)(1-S)} \quad (85)$$

$$= \frac{-8\pi/b^3}{4S} \cdot \frac{-2S}{(1-S^2)} \quad (86)$$

$$= \frac{4\pi}{b^3(1-S^2)} \quad (87)$$

$$= \frac{4\pi}{b^3[1 - (1 - 4\frac{a^2}{b^2})]} \quad (88)$$

$$= \frac{4\pi}{b^3 \cdot 4\frac{a^2}{b^2}} \quad (89)$$

$$= \frac{\pi}{ba^2} \quad (90)$$

Hooray!

5.2.2 Critically damped

Our factored function $f(z)$ is

$$f(z) = \frac{1}{(z - z_{r+})^2(z - z_{r-})^2} \quad (91)$$

Applying eq. 63 and 65 we have

$$I = 2\pi i \text{Res}(z = z_{r+}, f(z)) \quad (92)$$

$$= 2\pi i \left(\frac{1}{2!} \lim_{z \rightarrow z_{r+}} \frac{d}{dz} \frac{1}{(z + z_{r+})^2} \right) \quad (93)$$

$$= \pi i \lim_{z \rightarrow z_{r+}} -2 \cdot \frac{1}{(z_{r+} + z_{r+})^3} \quad (94)$$

$$= -2\pi i \frac{1}{z_{r+}^3} \quad (95)$$

$$= -2\pi i \frac{1}{\left(\frac{ib}{2}\right)^3} \quad (96)$$

$$= \frac{\pi}{b\left(\frac{b}{2}\right)^2} \quad (97)$$

$$= \frac{\pi}{ba^2}, \quad (98)$$

which matches eq. 90

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 or derive it for yourself in about three lines :p.
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