Thermodynamic Behaviour of Acoustic Modes

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Introduction

Thermodynamics provides a physical description of systems with a relatively large number of subsystems with hidden degrees of freedom. In this broad sense the theory is applicable to subsystems, such as constitutive particles, with well defined boundaries as well as quantum particles defined in terms of states [1]. In this work we utilize the formal analogy between determinate quantum states [2] and classical acoustic modes to treat sound fields thermodynamically. The approach is expected to be useful when the modes cannot (or need not) be determined exactly. In fact, it has already been noted in literature [3][4] that the flow of sound energy in the statistical energy analysis (SEA) is equivalent to the flow of heat in the state of (classical) canonical thermodynamic equilibrium with maximal entropy. As an extension of this finding, we treat non-diffuse sound fields as lower-entropy states and derive a simple correction of sound pressure level obtained using the statistical theory.

In addition to this, a fundamental result of quantum thermodynamics is used to derive the standard equation of state for the considered homentropic background ideal gas, by assigning acoustic-like modes to the fluid particles. The demonstrated alternative approach appears to be more natural in the acoustic context, since it does not require an external thermodynamic theory of the fluid or a different formalism.

Quantum determinate states as eigenmodes

The analogy between classical acoustics and quantum mechanics follows from the formal equivalence of the Helmholtz equation and the time-independent Schrödinger equation in a three-dimensional space,

$$\frac{2M_\psi E}{\hbar^2}\psi + \nabla^2\psi - \frac{2M_\psi}{\hbar^2}V\psi = 0, \tag{1}$$

with $\psi(\vec{x})$ quantum determinate state of energy E, M_ψ particle mass, $\hbar$ reduced Planck constant, and V real potential function. For $V = 0$ in vacuum (which corresponds to the background fluid) and $2M_\psi = m$, the equation takes the form of the Helmholtz equation:

$$\frac{Em}{\hbar^2}\psi + \nabla^2\psi = 0. \tag{2}$$

The omitted potential term depends on the particle's environment and can be associated with boundary conditions. Thus, quantum states ψ with eigenvalues $E = \omega^2\hbar^2/(mc_0^2)$ correspond to acoustic modes for c_0 the speed of sound and ω angular frequency. Moreover, in addition to purely acoustic modes ψ, we introduce non-acoustic modes ψ_0 associated with the background fluid. This allows an essentially equal treatment of the background fluid and in the following both types of modes will be treated thermodynamically.

The fundamental property of eigenvectors is orthogonality:

$$\int_{V_S} \psi_m^*(\vec{x})\psi_n(\vec{x})d^3\vec{x} = \begin{cases} NM & \text{for } m = n \\ 0 & \text{otherwise,} \end{cases} \tag{3}$$

where the integration is over the entire volume V_S of a (bounded) space, m and n are positive integers, and * denotes complex conjugate. Here we introduced the total number of elementary particles in the determinate state ψ_n, N, and mass of a single particle, M. In the case of the background fluid, the latter is molecular mass M_0 and N is the total number of fluid molecules. For acoustic fields, we define phonons with mass $M = E/c_0^2 = \hbar\omega/c_0^2$. In both cases the particle mass is very small and the number of particles is much larger than one for any V_S. In quantum mechanics the eigenmodes are additionally normalized such that $NM = 1$ and $|\psi|^2$ expresses the probability density of a particle's location.

Thermodynamics of the background fluid

If the environment E of any particle consists of $N_{m,\mathrm{E}}$ fluid molecules as identical ultraweakly coupled sub-systems, the total energy equals

$$E_\mathrm{E} = \sum_{i=1}^{n} N_{m,\mathrm{E},i}E_{\mathrm{E},i} \tag{4}$$

while

$$\sum_{i=1}^{n} N_{m,\mathrm{E},i} = N_{m,\mathrm{E}}, \tag{5}$$

with n denoting the total number of bins (each characterized with an energy value $E_{\mathrm{E},i}$) and $N_{m,\mathrm{E},i}$ the number of molecules in the state with energy $E_{\mathrm{E},i}$. In view of the previous section, $E_{\mathrm{E},i} = \omega_i^2\hbar^2/(M_0c_0^2)$, so n represents the number of frequency bins given by ω_i, and $N_{m,\mathrm{E}} \gg 1$.

For a given E_E, the number of states in which the environment consisting of distinguishable molecules can be found is [2]

$$\mathcal{N}_{m,\mathrm{E}}(E_\mathrm{E}) = \frac{N_{m,\mathrm{E}}!}{\prod_{i=1}^{n}(N_{m,\mathrm{E},i}!/d_i^{N_{m,\mathrm{E},i}})}, \tag{6}$$

where d_i is degeneracy (number of modes belonging to the same bin). For large numbers $N_{m,\mathrm{E},i}$ Stirling's ap-

proximation gives

$$\begin{aligned}\ln(\mathcal{N}_{m,\mathrm{E}}(E_\mathrm{E})) &\approx N_{m,\mathrm{E}}\ln(N_{m,\mathrm{E}}) \\ &+\sum_{i=1}^{n}\left(N_{m,\mathrm{E},i}\ln(d_i)-N_{m,\mathrm{E},i}\ln(N_{m,\mathrm{E},i})\right).\end{aligned} \tag{7}$$

Canonical equilibrium is defined as a configuration of E for which maximal number of bins are occupied. The method of Lagrange multipliers applied for maximizing $\ln(\mathcal{N}_{m,\mathrm{E}}(E_\mathrm{E}))$ under the conditions in equations (4) and (5) gives

$$\begin{aligned}&\frac{\partial}{\partial N_{m,\mathrm{E},i}}\left(\ln(\mathcal{N}_{m,\mathrm{E}}(E_\mathrm{E}))+\alpha\left(N_{m,\mathrm{E}}-\sum_{i=1}^{n}N_{m,\mathrm{E},i}\right)\right) \\ &\quad+\frac{\partial}{\partial N_{m,\mathrm{E},i}}\left(\beta\left(E_\mathrm{E}-\sum_{i=1}^{n}N_{m,\mathrm{E},i}E_{\mathrm{E},i}\right)\right) \\ &\quad\approx\ln(d_i)-\ln(N_{m,\mathrm{E},i})-\alpha-\beta E_{\mathrm{E},i}=0\end{aligned} \tag{8}$$

and the Boltzmann-Gibbs distribution as the solution [2]:

$$N_{m,\mathrm{E},i}=d_i e^{-\alpha-\beta E_{\mathrm{E},i}}=d_i e^{-\alpha-E_{\mathrm{E},i}/(k_B T_0)}, \tag{9}$$

where α and β are the Lagrange multipliers and the equilibrium temperature is defined as $T_0=1/(\beta k_B)$ with k_B the Boltzmann constant.

The exact values of d_i and $E_{\mathrm{E},i}$ depend on the potential of the environment. If the molecules are located in a three-dimensional infinite square well (which is analogous to a rectangular room or cavity with fully reflecting walls) with volume V_S and we let large ω_i take continuous positive values ω, then [2][5]

$$d=\frac{V_S}{2\pi^2 c_0^3}\omega^2 d\omega. \tag{10}$$

Moreover, it can be shown that the equality holds in acoustically large rooms regardless of their shapes, when $\omega L/c_0 \gg 1$, with $L\sim\sqrt[3]{V_S}$ characteristic length scale of the room, so the oblique room modes prevail. Thus, the environment does not necessarily have to build a rectangular lattice.

After also replacing $E_{\mathrm{E},i}$ with continuous $\omega^2\hbar^2/(M_0c_0^2)$ and letting the highest frequency approach the infinity,

$$\begin{aligned}N_{m,\mathrm{E}}&=\frac{V_S e^{-\alpha}}{2\pi^2 c_0^3}\int_0^\infty e^{-\omega^2\hbar^2/(k_B T_0 M_0 c_0^2)}\omega^2 d\omega \\ &=V_S e^{-\alpha}\left(\frac{k_B T_0 M_0}{4\pi\hbar^2}\right)^{3/2}\end{aligned} \tag{11}$$

and

$$\begin{aligned}E_\mathrm{E}&=\frac{V_S e^{-\alpha}\hbar^2}{2\pi^2 M_0 c_0^5}\int_0^\infty e^{-\omega^2\hbar^2/(k_B T_0 M_0 c_0^2)}\omega^4 d\omega \\ &=\frac{3N_{m,\mathrm{E}}k_B T_0}{2}.\end{aligned} \tag{12}$$

The values of integrals hold for any ω in the upper limit of the integral which satisfies $\omega^2\hbar^2/(k_B T_0 M_0 c_0^2)\gtrapprox 4$. Together with $E_{\mathrm{E},i}=\omega_i^2\hbar^2/(M_0c_0^2)$ and the equation of state (13) which we are about to derive, this condition is automatically satisfied when $N_{m,\mathrm{E},i}\gg 1$, which was already assumed in Stirling's approximation. This shows that for the modal density in eq. (10) at high enough frequencies all eigenvalues $E_{\mathrm{E},i}$ (or ω_i) are equally probable. Not only is the maximal number of bins occupied, but they are also equally likely and the entropy is thus maximal. The same holds for room modes in a diffuse sound field, when no single mode dominates in the frequency response, which is in agreement with the findings in literature [3][4].

Equation (12) represents the expression for average kinetic energy of $N_{m,\mathrm{E}}$ atoms of an ideal monoatomic gas. The factor of 3 is due to the three degrees of freedom per atom [1], which belong to the same sub-system (here fluid molecule) and the factor of 1/2 is due to the supposed $m=2M_\psi$ in eq. (2), that is, $E_\mathrm{E}=3M_{\psi,\mathrm{E}}c_0^2=3N_{m,\mathrm{E}}M_0c_0^2/2$. With $2E_\mathrm{E}/(3N_{m,\mathrm{E}})=M_0c_0^2$ divided with the heat capacity ratio γ, we obtain the equation of state,

$$M_0c_0^2=\gamma k_B T_0. \tag{13}$$

Thus, thermodynamic behaviour of the steady background fluid, typically quiescent air, is completely determined by the large number of modes and molecules per mode. The mean density follows from the massive-field theory in combination with thermodynamic equilibrium condition and ultraweak interaction of molecules with their environment. In particular, d_i in eq. (9) was derived from the modal analysis of the field, while the exponential distribution was a result of the statistical treatment and supposed state of maximal entropy (the canonical equilibrium).

Thermodynamics of acoustic modes

In order to treat non-diffuse acoustic fields as non-equilibrium states (with entropy lower than the maximal), we define acoustic entropy. In a frequency band $\Delta\omega_\mathrm{band}$ (typically an octave or third-octave band) divided into small frequency bins $\Delta\omega_i$ $(i=1,2...n)$ it equals

$$S=-k_B\sum_{i=1}^{n}\frac{\mathrm{p}_i^2}{\sum_{j=1}^{n}\mathrm{p}_j^2}\ln\frac{\mathrm{p}_i^2}{\sum_{j=1}^{n}\mathrm{p}_j^2}, \tag{14}$$

where p_i^2 is mean squared sound pressure amplitude per hertz in the bin i. Due to normalization with $\sum_{j=1}^{n}\mathrm{p}_j^2$, the two fractions can be seen as the probability of a determinate state i and S is the Gibbs entropy. Furthermore, any first-order acoustic scalar can replace sound pressure. If $\mathrm{p}_i^2=\mathrm{p}_\mathrm{diff}^2$ is equal for every i, the entropy is maximal, $S_\mathrm{diff}=k_B\ln(n)$. This is the case with a diffuse field and, as already noticed in literature [4] and the previous section, diffuse field is the analogue state of canonical thermodynamic equilibrium at high frequencies. If $\mathrm{p}_i^2\neq 0$ for a single value of i, the entropy is minimal, $S_\mathrm{min}=0$, because in this frequency bin $\mathrm{p}_i^2=\sum_{j=1}^{n}\mathrm{p}_j^2$. Hence, the acoustic entropy quantifies "tonality" of the power spectral density.

Still, additional care is necessary when using power spectra for an acoustically meaningful entropy. In principle, each mode (determinate state) should be associated

only with the frequency bin containing its eigenfrequency. However, if the bins are too narrow, damped acoustic modes with finite widths can extend over several adjacent bins. On the other hand, if the bins are too wide, details of power spectra are not captured well and the thermodynamic approximation becomes too crude. As a reasonable compromise, we first assume that the damping constant $\zeta_i = \zeta$ is equal for all modes and bins i in the considered frequency band $\Delta f_{\mathrm{band}} = \Delta\omega_{\mathrm{band}}/(2\pi)$, which is divided into n equally wide and non-overlapping frequency bins $\Delta f_i = \Delta\omega_i/(2\pi) = \Delta f_{\mathrm{band}}/n$. In other words, the frequency bands are chosen such that the damping (or reverberation time in a room) does not vary significantly within each band. Then we set the bin width equal to the half-width of the modes [5], $\Delta\omega_i = 2\zeta_i$.

Within the range $\Delta\omega_i$ centred at a mode's eigenfrequency, energy of the mode drops 50% with respect to its peak value. The thermodynamic analogy thus becomes inadequate if modes overlap and interfere significantly, such that amplitudes of different modes are comparable within $\Delta\omega_i$. This is the case at high frequencies (above the Schroeder frequency), when the classical SEA is more suitable. It is also invalid when $\Delta\omega_i$ is comparable to $\Delta\omega_{\mathrm{band}}$, such as for very damped rooms at low frequencies. The analogy is thus relevant in frequency range around the Schroeder frequency, where distinct modes are not dominant, but the number of modes per bin is not high enough for the statistical theory.

While entropy can be calculated from power spectra, it is of interest to estimate it analytically. In order to obtain a simple solution, we suppose that all modes are equally excited and all m ($m \leq n$) non-zero values of p_i^2 are equal, $\mathrm{p}_i^2 = \mathrm{p}^2$. Thus, m is the number of bins with excited modes and the entropy simplifies to

$$S = -k_B \ln \frac{\mathrm{p}^2}{m\mathrm{p}^2} = k_B \ln(m). \tag{15}$$

Under the assumption that only one mode can dominate in a single frequency bin, m represents the number of modes in $\Delta\omega_{\mathrm{band}}$. At high frequencies, when many modes overlap in frequency bins and the analogy becomes inaccurate, the number of modes can surpass the number of bins, leading to $S > S_{\mathrm{diff}}$. At such frequencies $S = S_{\mathrm{diff}}$ must be forced and the analogy reduces to SEA.

From eq. (15) with $m\mathrm{p}^2 = n\mathrm{p}_{\mathrm{diff}}^2$ (for comparison with a diffuse field with equal total energy in $\Delta\omega_{\mathrm{band}}$), $S = S_{\mathrm{diff}} - k_B \ln\left(\mathrm{p}^2/\mathrm{p}_{\mathrm{diff}}^2\right)$. For $m \leq n$, $\mathrm{p}^2 \geq \mathrm{p}_{\mathrm{diff}}^2$ and the non-negative sound pressure level difference $\Delta L = 10\log_{10}(\mathrm{p}^2/\mathrm{p}_{\mathrm{diff}}^2)$ can be estimated and used as a correction of the diffuse-field value obtained, for example, with the standard SEA. The correction amounts to the entropy difference between diffuse and non-diffuse field:

$$\Delta L = (10\log_{10} e)\frac{S_{\mathrm{diff}} - S}{k_B} = (10\log_{10} e)\left(\ln n - \frac{S}{k_B}\right). \tag{16}$$

For $m \approx n$ the correction is most accurate, while for $m \ll n$ it merely indicates the contribution of strong peaks in the spectrum. Importantly, the constant k_B from the definition of entropy cancels out and does not affect the value of ΔL.

For a simple and crude estimation of entropy from eq. (15) in rectangular rooms, the number of modes m can be calculated using more accurate extension of eq. (10) which includes axial and tangential modes [5],

$$d = \sum_{i=1}^{n}\left(\frac{V_S\omega_i^2}{2\pi^2 c_0^3} + \frac{S_S\omega_i}{8\pi c_0^2} + \frac{L_S}{16\pi c_0}\right)\Delta\omega_i, \tag{17}$$

with $V_S = L_1L_2L_3$, $S_S = 2(L_1L_2 + L_2L_3 + L_1L_3)$, $L_S = 4(L_1 + L_2 + L_3)$, L_1, L_2, and L_3 dimensions of the room, and ω_i the centre frequency of $\Delta\omega_i$. Since $d/\Delta f_{\mathrm{band}} = m/(n \cdot 1\,\mathrm{Hz})$ represents modal density (number of modes per hertz, recalling that maximum one mode is expected to dominate in a single frequency bin),

$$m = nd\frac{1\,\mathrm{Hz}}{\Delta f_{\mathrm{band}}} = d\frac{1\,\mathrm{Hz}}{\Delta f_i}. \tag{18}$$

In general this gives a real value of m, rather than an integer number of modes in eq. (15). However, for a large number of modes in the frequency band, the rounding has no significant effect. At the lowest frequencies, when m is comparable to or smaller than one, the thermodynamic analogy is not valid anyway (the wave equation could be solved numerically). Formally, $\Delta L = 0$ can be set for $d < 1/3$, assuming a flat power spectrum well below the lowest eigenfrequency. As already discussed, we also set $S = S_{\mathrm{diff}} = k_B \ln n$ and therefore $\Delta L = 0$ for $m > n$.

Figure 1 shows the calculated average sound pressure level in a rectangular room with dimensions (L_1, L_2, L_3) = (5 m, 4 m, 3 m) filled with air at room temperature (c_0 = 343 m/s, ρ_0 = 1.2 kg/m^3). The considered frequency range $(f_{\min}, f_{\max})$ = (10 Hz, 7130 Hz) is divided into the standard third-octave bands and frequency bins $\Delta f_i = \Delta f = \zeta/\pi$ with [5] $\zeta = 3\ln(10)/T_{60}$. For simplicity, reverberation time T_{60} is frequency-independent and three values are considered: 0.5 s, 2 s, and 8 s. Sound energy density per hertz in the diffuse field is calculated as [5]

$$E_{\mathrm{diff},i} = \frac{4P_W}{c_0 A} \tag{19}$$

with acoustic power of the source per hertz $P_W = (Q^2/1\mathrm{Hz})/(8\pi\rho_0 c_0)$, unit source strength Q = 1 kg/s^2, and the equivalent absorption area is estimated using Sabine's formula, $A = (8\zeta V_S)/c_0$.

Mean squared sound pressure amplitude per hertz in each bin i is estimated as [5]

$$\mathrm{p}_i^2 = \frac{Q^2/1\mathrm{Hz}}{C_s^2}\left|\frac{8c_0^2}{V_S}\sum_s \frac{\prod_{j=1}^{3}\cos(k_{sj}x_j)\prod_{l=1}^{3}\cos(k_{sl}y_l)}{\omega_s^2 + 2j\zeta_s\omega_s - \omega_i^2}\right|^2, \tag{20}$$

with $\zeta_s = \zeta$ for each mode s. The eigenfrequencies $\omega_s = k_s c_0$ are calculated using $k_s = \sqrt{k_{s1}^2 + k_{s2}^2 + k_{s3}^2} = \sqrt{(s_1\pi/L_1)^2 + (s_2\pi/L_2)^2 + (s_3\pi/L_3)^2}$, where s_1, s_2, and

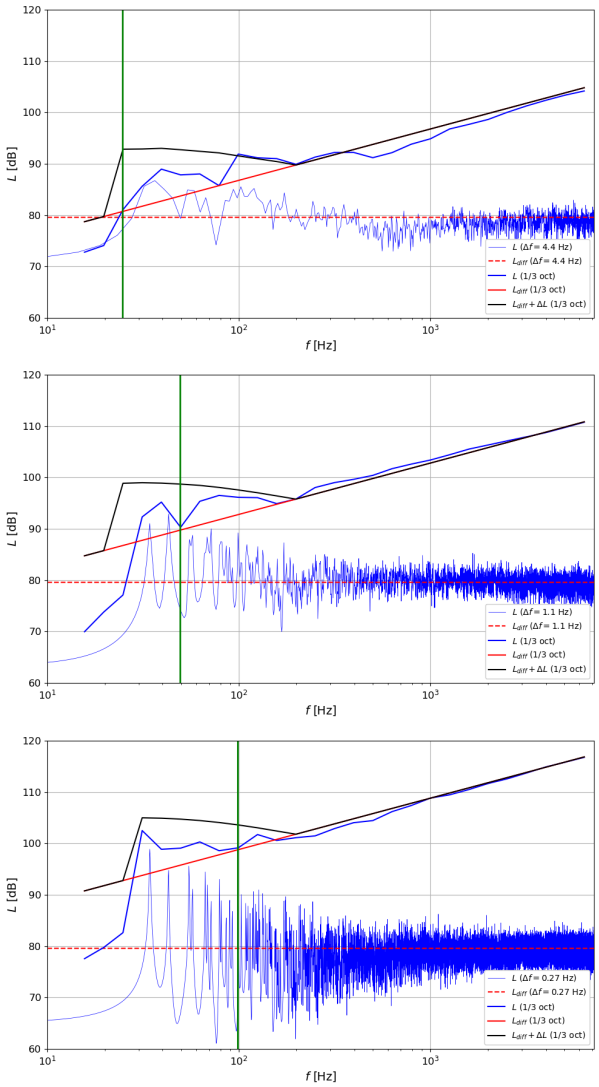

Figure 1: Average sound pressure level in the rectangular room with reverberation time (top) 0.5 s, (middle) 2 s, and (bottom) 8 s.

s_3 are non-negative integers, and C_s equals 4 for single $s_i \neq 0$ (axial modes), 2 for two $s_i \neq 0$ (tangential modes), or 1 for all three $s_i \neq 0$ (oblique modes). Apart from the non-acoustic mode $(s_1, s_2, s_3) = (0, 0, 0)$, all modes with $\omega_s/(2\pi) \leq 1.1 f_{\max}$ are included in the sum in eq. (20). The values of p_i^2 are averaged over ten different pairs of source ($\vec{y}$) and receiver ($\vec{x}$) locations with the components (y_1, y_2, y_3) and (x_1, x_2, x_3), respectively, taken independently from the uniform distributions in the ranges (0, L_1), (0, L_2), and (0, L_3). The average sound energy density per hertz is then expressed with

$$E_i = \frac{\mathrm{p}_i^2}{2\rho_0 c_0^2}. \tag{21}$$

Both for the diffuse-field estimation using eq. (19) (L_{diff}) and spectra obtained using eq. (21) (L), sound pressure level in the bin i is calculated as

$$L_i = 10 \log_{10} \frac{E_i \Delta\omega_i c_0}{2\pi p_{\mathrm{ref}}^2/(\rho_0 c_0)}, \tag{22}$$

with $p_{\mathrm{ref}} = 2{\cdot}10^{-5}$ Pa. In the case of a diffuse field, $\Delta\omega_i/2$ cancels with $\zeta = \Delta\omega_i/2$ from Sabine's formula, leading to the values of $L_{\mathrm{diff},i}$ independent of the reverberation time. The third-octave values are obtained by means of energy summation, $L_{1/3\ \mathrm{oct}} = 10 \log_{10} \left(\sum_i 10^{L_i/10}\right)$, where the sum is over all bins belonging to the third-octave band. Correction of the diffuse-field value, ΔL, is calculated using eq. (16) and the entropy from equations (15), (17), and (18). The constant k_B does not affect its value and it is set to 1. The vertical green line in Fig. 1 indicates the Schroeder frequency estimated with the formula [5] $f_{\mathrm{Schroed}} = \sqrt{(3c_0^3)/(4\zeta V_S)}$.

The introduced correction captures well the increasing sound pressure level at frequencies around and below the Schroeder frequency, which is due to decreasing modal density. However, this is not the case at very low frequencies, when a few lowest modes determine the values of the spectrum. The simple correction based on the statistical treatment is not valid for such cases corresponding to very low entropy states, far from the canonical equilibrium. The thermodynamic approach is inadequate and the sound fields have to be calculated by other means, for example by solving the wave equation.

Conclusion

The analysis above showed that the equation of state of the background ideal gas can be derived by modelling the fluid molecules as quantum particles with associated acoustic-like modes and in the canonical equilibrium state. The equilibrium corresponds to a diffuse sound field. Both non-acoustic and classical acoustic modes are analogue to (non-normalized) determinate quantum states. The associated elementary particles are, respectively, fluid molecules and phonons (with mass $M = \hbar\omega/c_0^2$, by definition). Complementing the equilibrium state of diffuse fields, acoustic entropy (with appropriate bin width) is a measure of randomness/tonality in a given frequency band. The entropy difference between a diffuse and non-diffuse field can be used for introducing a correction of the statistical theory of sound fields in rooms at frequencies around the Schroeder frequency. Although this was demonstrated here primarily on sound fields in rooms, similar considerations are expected to be applicable for fields in solids, as well.

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