Zero-point energy: the idea underlying the quantum

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T. H. Boyer, Am. J. Phys. **71**, 866 (2003):

By a thermodynamic analysis of the harmonic oscillator Boyer finds:

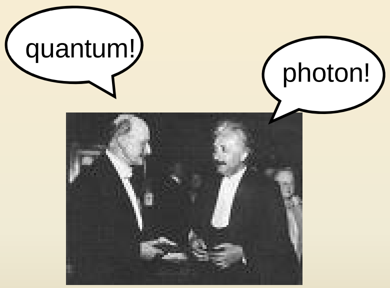
$$U(\omega,T) = \omega f(\omega/T) \xrightarrow[T=0]{} U(\omega,0) \equiv E_0 = \text{const}\cdot\omega \longrightarrow$$

Wien's law — Zero-point energy — Breakdown of equipartition!! $U = kT$

The existence of a zero-point energy emerges **naturally** from the thermodynamic relations and breaks down with classical physics…

How far can we get by introducing this new (non-classical) physical element into the statistical description of a system of harmonic oscillators?

The results obtained coincide with those that led Planck and Einstein to establish the quantum hypothesis of the radiation field.



OUTLINE

- Thermodynamic and statistical description of the harmonic oscillator

  Introduction the zero-point energy into the statistical description

- Establishing Planck's law

  Derivation of Planck's law from the statistical information

- Discussion: the quantum hypothesis of Planck and Einstein

  Historical overview and comparison of Einstein's analysis with the present approach

- Continuous *vs* discrete

  Disclosing the origin of discreteness

- Non-thermal fluctuations

  Introduction of the zero-point energy fluctuations into the description

- Concluding remarks

Statistical information

The statistical information of the system is contained in a distribution function W from which the mean values of any function $f(E)$ can be calculated:

$$\overline{f(E)} = \int W(E) f(E)\, dE \qquad \bar{E} = U(T) = U$$

Moreover, W is such that it maximizes the entropy defined as

$$S = -k \int W \ln W \, dE$$

Such distribution can be expressed as (Montroll and Shlesinger, Jour. Stat. Phys. **32**, 209 (1983))

$$W_g(E) = \frac{1}{Z_g(\beta)} g(E) e^{-\beta E}$$

with

$$Z_g(\beta) = \int g(E) e^{-\beta E} dE \qquad \beta = (kT)^{-1}$$

The choice $g(E)=1$ corresponds to $W_{g=1}(E)=\frac{1}{Z_1(\beta)}e^{-\beta E}$, and leads to

$$\bar{E}=U=kT$$

Equipartition and inconsistency with some of Boyer's relations

Thus in order to account for a zpe a more general function $g(E)$ is needed.

- Thermal fluctuations

For the general distribution W_g the following recurrence relation holds (r a positive integer)

$$\overline{E^{r+1}}=U\overline{E^{r}}-d\overline{E^{r}}/d\beta$$

In particular, for the dispersion of the energy,

$$\sigma_E^2\equiv\overline{(E-U)^2}=\overline{E^2}-U^2$$

we obtain

$$\sigma_E^2=-dU/d\beta=kT^2C_v\ \xrightarrow{T=0}\ \sigma_E^2(T=0)=0$$

fluctuations are of thermal nature

Establishing Planck's law

Knowing σ_E^2 as a function of U determines $U(\beta)$

$$-d\beta = \frac{dU}{\sigma_E^2(U)}, \qquad \sigma_E^2(E_0) = 0$$

- Determination of the dispersion as a function of U

$$\sigma_E^2 = \overline{E^2} - \left(\overline{E}\right)^2$$

We expand σ_E^2 as a power series of U and note that for high temperatures the result $\sigma_E^2 = U^2$ must be recovered. Thus the dispersion reduces to a polynomial of second order in U:

$$\sigma_E^2(U) = a_0 + a_1 U + U^2$$

Since σ_E^2 is invariant under the transformation $E \to -E$ it follows that $\sigma_E^2(U) = \sigma_E^2(-U)$, thus

$$\sigma_E^2 = a_0 + U^2$$

And since $\sigma_E^2(E_0) = 0$ it follows that

$$\sigma_E^2 = U^2 - E_0^2$$

The equation

$$\frac{dU}{U^2 - E_0^2} = -d\vartheta$$

has the solution

$$\vartheta = \begin{cases} \dfrac{1}{U} & \text{for } E_0 = 0 \longrightarrow U(\vartheta) = \dfrac{1}{\vartheta} \\[2ex] \dfrac{1}{E_0}\coth^{-1}\dfrac{U}{E_0} & \text{for } E_0 \neq 0 \longrightarrow U(\vartheta) = E_0 \coth E_0 \vartheta \end{cases}$$

No zpe means equipartition

Zpe means Planck's law

The zero-point energy is a **necessary and sufficient** condition to arrive at Planck´s law…

(no quantum hypothesis is required)

$$U = U_T + E_0 \longrightarrow U_T = E_0 \coth E_0 \vartheta - E_0$$

Original result of Planck

Discussion: the quantum hypothesis of Planck and Einstein

$$\frac{\partial S}{\partial U_T} = \frac{1}{T}$$

- Planck´s analysis: the birth of the quantum

$T \to \infty$: $\quad \dfrac{\partial^2 S}{\partial U_T^2} = -\dfrac{k}{U_T^2}$

$T \to 0$, $U_T = 2\varepsilon_0 e^{-2\varepsilon_0/kT}$: $\quad \dfrac{\partial^2 S}{\partial U_T^2} = -\dfrac{k}{2\varepsilon_0 U_T}$

$$\frac{\partial^2 S}{\partial U_T^2} = -\frac{k}{U_T^2 + 2\varepsilon_0 U_T}$$

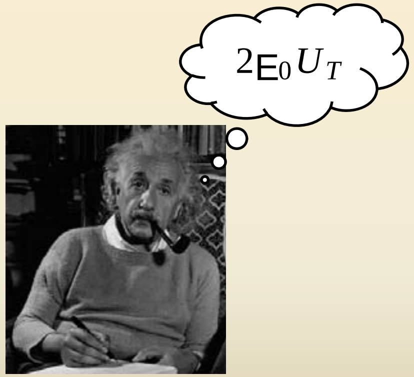
- Einstein´s analysis: the birth of the quantized radiation field

$$\frac{\partial^2 S}{\partial U_T^2} = -\frac{k}{U_T^2 + 2\varepsilon_0 U_T}$$

$$\frac{\partial^2 S}{\partial U_T^2} = \frac{\partial}{\partial U_T}\frac{1}{T} = -\frac{1}{T^2 C_v}$$

$$kT^2 C_v = -\frac{\partial U_T}{\partial \beta} = \sigma_\varepsilon^2$$

$$\sigma_\varepsilon^2 = U_T^2 + 2\varepsilon_0 U_T$$



$$\sigma_{\mathcal{E}}^2 = U_T^2 + 2\mathcal{E}_0 U_T$$

Fluctuations resulting from the interference among the modes of the thermal radiation field

Undulatory aspect of the radiation field

Fluctuations resulting from a poissonian process: independent events

Corpuscular aspect of the radiation field

No zpe is considered and a corpuscular property of the radiation field emerges

The present approach suggest an alternate interpretation: the fluctuations are due to the interferences of the thermal radiation field…

…among its own modes…

$$\sigma_{\mathcal{E}}^2 = \langle U^2 \rangle - \mathcal{E}_0^{\,2}, \quad U = U_T + \mathcal{E}_0 \longrightarrow \sigma_{\mathcal{E}}^2 = U_T^2 + 2\mathcal{E}_0 U_T$$

…and among its modes with those of the zero-point field.

Continuous *vs* discrete

Where is the connection between both approaches?

From the thermodynamic relations it can be shown that

$$U = -\frac{d \ln Z_g(\beta)}{d\beta}$$

With $U(\beta) = \varepsilon_0 \coth \varepsilon_0 \beta$ we obtain for the partition function:

$$Z_g(\beta) = \frac{2\varepsilon_0}{2 \sinh \varepsilon_0 \beta} = 2\varepsilon_0 \frac{e^{-\varepsilon_0 \beta}}{1 - e^{-2\varepsilon_0 \beta}} = 2\varepsilon_0 \sum_{n=0}^{\infty} e^{-\varepsilon_0 \beta (2n+1)} = 2\varepsilon_0 \sum_{n=0}^{\infty} e^{-\beta E_n}$$

$$E_n \equiv (2n+1)\varepsilon_0$$

The partition function is related to $g(E)$ by means of the expression

$$Z_g(\beta) = \int g(E)\, e^{-\beta E}\, dE = 2\varepsilon_0 \sum_{n=0}^{\infty} e^{-\beta E_n}$$

From which it follows that

$$g(E) = 2\varepsilon_0 \sum_{n=0}^{\infty} \delta(E - E_n)$$

Substituting $g(E)$ in the expression for the distribution function $W_g(E) = \frac{1}{Z_g(\beta)} g(E) e^{-\beta E}$ leads to

$$W_g(E) = \frac{1}{Z}\sum_{n=0}^{\infty} \delta(E - E_n) e^{-\beta E} \quad \text{where} \quad Z = \sum_{n=0}^{\infty} e^{-\beta E_n}$$

Therefore the mean value of any function $f(E)$ takes the form

$$\overline{f(E)} = \int W_g(E) f(E)\, dE = \frac{1}{Z}\sum_{n=0}^{\infty} f(E_n) e^{-\beta E_n} = \sum_{n=0}^{\infty} w_n f(E_n) \qquad w_n = \frac{1}{Z} e^{-\beta E_n}$$

Continuous description
Averages over the **continuous variable *E***

Discrete description
Averages over the **discrete states *n***

Since n characterizes the energy,

$$E_n = (2n+1)\mathcal{E}_0 ,$$

it seems natural to assign a discrete property to the energy though it may acquire continuous values (it fluctuates!). Those mean energies corresponding to the thermal equilibrium have a discrete spectrum.

Non-thermal fluctuations

- Including zero-point fluctuations

$$\langle \sigma_E^2 \rangle_{Thermal} = \sigma_E^2 = U_T^2 + 2E_0 U_T, \qquad \sigma_E^2(T=0) = 0$$

Fluctuations of *thermal* nature

The term representing the interference among the modes of the zpf is missing

$$\langle \sigma_E^2 \rangle_{Total} = U_T^2 + 2E_0 U_T + E_0^2 \qquad U = U_T + E_0 \;\longrightarrow\; \langle \sigma_E^2 \rangle_{Total} = U^2$$

The distribution W_g cannot account for *all* fluctuations, but only for the *thermal* ones. Thus we look for W_s such that

$$\langle \sigma_E^2 \rangle_s = U^2$$

This generalizes the result:

Relates *thermal* fluctuations with *thermal* energy

$$\langle \sigma_E^2 \rangle_{Thermal} = U_{Equipartition}^2$$

The distribution that satisfies this requirement and maximizes the entropy is

$$W_s(E) = \frac{1}{U} e^{-E/U}$$

It includes fluctuations beyond the thermal ones.

The corresponding entropy is then

$$S_s = -k \int W_s \ln W_s \, dE = k \ln U + k$$

Therefore,

$$\frac{\partial S_s}{\partial U} = \frac{k}{U} \quad \longleftrightarrow \quad \frac{\partial S_{Thermal}}{\partial U} = \frac{1}{T}$$

Planck and Einstein

Coincide only when the zpe is zero

Thus the existence of the zpe requires a more general (statistical rather than thermodynamic) entropy that should accomodate *all* fluctuations.

- Phase space description

The quadratures p, q of the harmonic oscillator are related to its energy according to

$$E = \left(p^2 + m^2 \omega^2 q^2\right)/2m$$

Noting that the energy distribution stands for a reduced probability density in the action-angle variables space,

$$W(E) = \int_0^{2\pi} W(E, \phi) \, d\phi$$

we can derive the probability density in the phase space (q,p) taking into account that

$$W(\mathcal{E},\omega)\,d\mathcal{E}\,d\omega = W(p,q)\,dp\,dq$$

The resulting probability density has the form

$$W(p,q)=\frac{\omega}{2\pi U}\exp\left(-\frac{p^2+m^2\omega^2 q^2}{2mU}\right)$$

Wigner function

$$U(\omega)=\mathcal{E}_0\coth\mathcal{E}_0/kT$$

W can be decomposed as the product of two gaussian distributions with variances

$$\sigma_p^2=mU \qquad \sigma_q^2=U/m\omega^2$$

$$\mathcal{E}_0=\hbar\omega/2$$

$$\sigma_q^2\sigma_p^2=\frac{U^2}{\omega^2}=\frac{1}{\omega^2}\left(\mathcal{E}_0^2+\sigma_{\mathcal{E}_T}^2\right)\geq\frac{\mathcal{E}_0^2}{\omega^2}=\frac{\hbar^2}{4}$$

$$\sigma_{\mathcal{E}}^2=U^2-\mathcal{E}_0^2$$

non-thermal fluctuations

thermal fluctuations

Quantum fluctuations are due to the fluctuations of the zpe

Concluding remarks

- Wien's law allows for a zero-point energy that breaks down with the classical (equipartition) result.
- This zero-point energy **unequivocally** determines Planck´s law. No explicit quantum hypothesis is needed.
- The **fluctuating** zero-point energy lies at the root of quantum fluctuations.
- Quantum theory could have been born from this notion (zpe physics).
- Does this physical element is richer?....